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1. DEGREE OF LOCALIZATION IN THREE-DIMENSIONAL DISORDEREDT
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2. SOME PHASE-THEORETICAL NOTES ON LOCALIZATION OF EIGENFUNCTIONS
   F. J. Hori Physics Department, Hokkaido University, Sapporo, Japan

3. THEORY OF LOCALISATION IN DISORDERED SYSTEMS
   T. Lukes Department of Applied Mathematics and Mathematical Physics, University College, Cardiff, U.K

4. SUMMARY OF THREE LECTURES ON POLARONS
   J. Devreese University of Antwerp, Belgium

DEGREE OF LOCALIZATION IN THREE-DIMENSIONAL DISORDERED SYSTEMS

by

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Abstract

It is shown that any matrix element of Green operator can be expanded in terms of principal minors of the secular determinant of the system under consideration. For diagonal elements the expansion turns out to be the same as Anderson's renormalized perturbation expansion of the self-energy. However, our method not only gives its much simpler derivation, but also discloses its more general physical and mathematical significance. Upon its basis, the interrelation between self-energies, principal minors of secular determinants, and the state ratios, which play an important role in the phase-theoretical treatment of the localization of eigenfunctions in disordered systems, is studied. From this it is concluded that in the case of diagonally-disordered one-dimensional system with nearest-neighbour interactions only, the state ratio and the self-energy are essentially the same quantities, and the degree of localization, defined in the phase theory in terms of the state ratio, can be defined also in terms of the self-energy. Secondly, it is shown, on the basis of the expansion of off-diagonal elements of Green operator, that in one-dimensional case the degree of localization thus defined gives the exponent of average exponential decay of Green's function. From this it is concluded that it is reasonable to define the degree of localization in three-dimensional disordered systems by the exponent of average exponential decay of Green's function. Thirdly, it is shown that, in diagonally-disordered three-dimensional systems with nearest-neighbour interactions only, the degree of localization defined in this way can be bounded by two functions $-\ln f(E)$ and $-\ln g(E)$, where $f(E)$ and $g(E)$ are the functions which give the criterion of convergence of the renormalized perturbation expansion and the series of the first terms of the expansions of off-diagonal elements of Green operator, respectively. From this it can be concluded that under certain conditions the phase-theoretical concept of localization agrees with that in Anderson's theory.

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0. Introduction

The problem of localization of eigenfunctions in disordered systems has been discussed from two different points of view. One is the phase-theoretical argument, which was originated from the classical papers of Mott and Twose[1] and Roberts and Makinson[2], and formulated more rigorously by Borland[3], Halperin[4], Matsuda and Ishii[5], Hori and Minami[6] [7], and Tong[8]. The other is what was given by Anderson[9], which was later examined in more detail by Thouless[10] and Economou and Cohen[11]. The former approach is mathematically more sound than the second, but has a demerit that it can give significant results only for one-dimensional systems. The latter is based on a series of physical arguments which involve several subtle or ambiguous points, but is free from the restriction of dimensionality. It is highly desirable to fill the gap between these two approaches and to formulate a unified theory which is mathematically rigorous and at the same time has no dimensional handicap. This gap cannot be filled, however, by simply trying to generalize the phase-theoretical treatment to multidimensional cases or to make the argument in Anderson's approach more rigorous. This is because the difference between these approaches is not merely in mathematical rigorousness, but is more profound. The most essential difference lies in the definition of localization. In the phase-theoretical treatment, the degree of localization $\overline{L}(E)$ is defined in terms of state ratio, and is believed to give the negative of the exponent of the exponential envelope of localized eigenfunction. In Anderson's theory the localization is defined by the absence of diffusion or the convergence of renormalized perturbation expansion (RPE) of the self-energy. According to Thouless and Economou and Cohen, there exists a function $f(E)$ such that if $f(E) < 1$ RPE converges and the eigenfunction is localized. The function $f(E)$ is defined in terms of self-energies. The main purpose of the present paper is to discuss, as the first step towards the formulation of a unified theory, the relation between these different concepts of localization.

For this purpose we first establish in paragraph 1 the general expansion formulas for diagonal as well as non-diagonal matrix elements of Green operator in terms of principal minors of its

secular determinant. For the diagonal elements, the expansion turns out to be just Anderson's RPE of the self-energy. However, our method is independent of any specific physical model, and not only gives a much simpler derivation of RPE, but also discloses its more general mathematical significance. On the other hand, the expansion of off-diagonal elements is new, as far as the authors are aware. It turns out to be very useful in bridging the gap between two different theories mentioned above.

In paragraph 2 we consider the special case of diagonally disordered one-dimensional system with nearest-neighbour interactions only and study, upon the basis of the expansion of diagonal elements of Green operator, the interrelation between self-energies, principal minors of secular determinants, and state ratios. It turns out that in the one-dimensional case, there is a very simple relation between these three quantities, so that the degree of localization $\acute{L}(E)$ can be expressed in terms of self-energies. Next it is shown, on the basis of the expansion of off-diagonal elements of Green operator, that in the one-dimensional case the degree of localization gives the exponent of average exponential decay of Green's function with the distance from a fixed site. This shows that we can naturally define the degree of localization in multidimensional disordered systems as the exponent of average exponential decay of Green's function. Finally it is shown, in paragraph 3, upon the basis of the above-mentioned two expansions, that in the case of diagonally disordered three-dimensional systems with nearest-neighbour interactions only, the degree of localization thus defined can be bounded by two functions $-\ln f(E)$ and $-\ln g(E)$, where $f(E)$ and $g(E)$ are functions which give the criterion of convergence of RPE and the series of the first terms of the expansions of non-diagonal elements of Green operator, respectively. From this it can be concluded that under certain conditions the phase-theoretical concept of localization agrees with that in Anderson's theory.

1. Expansion of Diagonal and Off-Diagonal Elements of Green Operator.

Let us begin from the following

THEOREM Determinanet A of any infinite-dimensional matrix $\mathbb{A}$ can be developed in terms of its principal minors:

$$A = a_{i_1 i_1} A^{i_1} + \sum_{m=2}^{\infty} \sum_{(i_2 i_3 \cdots i_m)}{}' (-1)^{m-1} a_{i_1 i_2} a_{i_2 i_3} \cdots a_{i_m i_1} A^{i_1 i_2 i_3 \cdots i_m}, \tag{1.1}$$

where $A^{i_1 i_2 \cdots i_m}$ is the principal minor which is obtained by deleting from A the $i_1 th$, $i_2 th$, $\cdots$, and i_mth rows and columns, and the prime means that the sum must be carried out only over all the sets of distinct indices $i_2, i_3, \cdots, i_m$, all of which are distinct from i_1.

Proof. First we expand A with respect to the i_1th row:

$$A = \sum_{i_2=1}^{\infty} a_{i_1 i_2} A_{i_1 i_2} = a_{i_1 i_2} A_{i_1 i_2} + \sum_{\substack{i_2=1 \\ i_2 \neq i_1}}^{\infty} a_{i_1 i_2} A_{i_1 i_2}, \tag{1.2}$$

where $A_{i_1 i_2}$ is the cofactor of the element $a_{i_1 i_2}$. Each cofactor can be expanded with respect to the i_2th row:

$$\begin{aligned} A_{i_1 i_2} &= \sum_{\substack{i_3=1 \\ i_3 \neq i_2}}^{\infty}{}' a_{i_2 i_3} A_{i_1 i_2 ; i_2 i_3} \\ &= a_{i_2 i_1} A_{i_1 i_2 ; i_2 i_1} + \sum_{\substack{i_3=1 \\ i_3 \neq i_1, i_2}}^{\infty}{}' a_{i_2 i_3} A_{i_1 i_2 ; i_2 i_3} . \end{aligned} \tag{1.3}$$

The cofactors $A_{i_1 i_2 ; i_2 i_3}$ appeared here can again be expanded as

$$\begin{aligned} A_{i_1 i_2 ; i_2 i_3} &= \sum_{\substack{i_4=1 \\ i_4 \neq i_3}}^{\infty}{}' a_{i_3 i_4} A_{i_1 i_2 ; i_2 i_3 ; i_3 i_4} \\ &= a_{i_3 i_1} A_{i_1 i_2 ; i_2 i_3 ; i_3 i_1} + \sum_{\substack{i_4=1 \\ i_4 \neq i_3, i_1}}^{\infty}{}' a_{i_3 i_4} A_{i_1 i_2 ; i_2 i_3 ; i_3 i_4}, \end{aligned} \tag{1.4}$$

and so on. Thus we obtain an expansion

$$A = a_{i_1 i_1} A_{i_1 i_1} + \sum_{m=2}^{\infty} \sum_{(i_1 i_2 \cdots i_m)}{}' a_{i_1 i_2} a_{i_2 i_3} \cdots a_{i_m i_1} A_{i_1 i_2 ; i_2 i_3 ; \cdots ; i_{m-1} i_m ; i_m i_1} \tag{1.5}$$

We now have only to replace each $A_{i_1 i_2 ; i_2 i_3 ; \cdots ; i_{m-1} i_m ; i_m i_1}$ by corresponding principal minors $A^{i_1 i_2 \cdots i_m}$, by attaching the appropriate sign to it. This sign can be determined easily. The sign of A^{i_1} must be $(-1)^{i_1+i_1} = 1$. The sign of $A^{i_1 i_2}$ can be determined as follows: First delete the i_1th row and the i_2th column to obtain the minor $A^{(i_1 i_2)}$, which is equal to $(-1)^{i_1+i_2} A_{i_1 i_2}$. Next delete the i_2th row and the i_1th column. Then we have (Fig. 1)

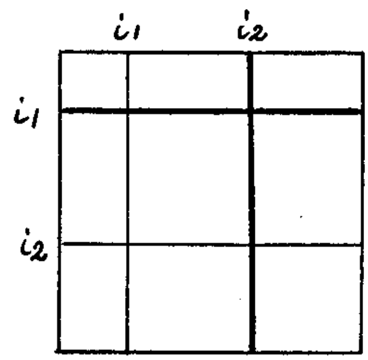

Fig. 1

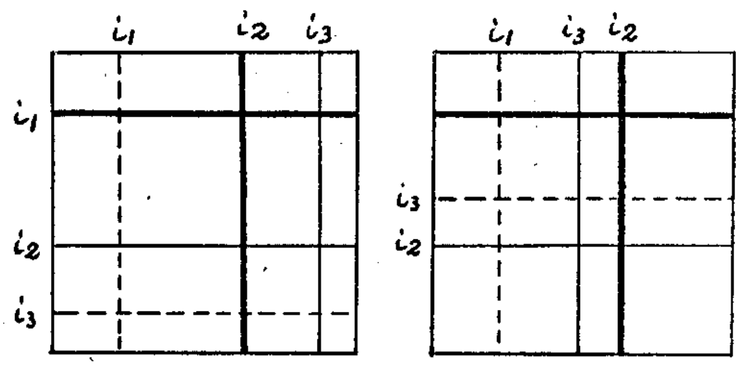

Fig. 2

The sign of $A^{i_1 i_2 i_3}$ may be determined in the same way: First delete from $A^{(i_1 i_2)}$ the i_2th row and the i_3th column to obtain the minor (Fig. 2)

$$A^{(i_1 i_3) i_2} = (-1)^{i_2+i_3} A^{(i_1 i_2)}_{i_2 i_3} \qquad i_3 > i_2$$

$$= (-1)^{i_2+i_3-1} A^{(i_1 i_2)}_{i_2 i_3} \qquad i_3 < i_2 .$$

Next delete the i_3 th row and the i_1 th column. Then we have

$$A^{i_1 i_2 i_3} = (-1)^{i_1+i_3} A^{(i_1 i_3) i_2}_{i_3 i_1} = (-1)^{i_1+i_3} (-1)^{i_2+i_3} A^{(i_1 i_2)}_{i_2 i_3 ; i_3 i_1}$$

$$= (-1)^{i_1+i_2} (-1)^{i_1+i_2} A_{i_1 i_2 ; i_2 i_3 ; i_3 i_1}, \qquad i_3 > i_2$$

$$= (-1)^{i_1+i_3-1} A^{(i_1 i_3) i_2}_{i_3 i_1} = (-1)^{i_1+i_3-1} (-1)^{i_2+i_3-1} A^{(i_1 i_2)}_{i_2 i_3 ; i_3 i_1}$$

$$= (-1)^{i_1+i_2} (-1)^{i_1+i_2} A_{i_1 i_2 ; i_2 i_3 ; i_3 i_1} \qquad i_3 < i_2$$

or

$$A^{i_1 i_2 i_3} = A_{i_1 i_2 ; i_2 i_3 ; i_3 i_1}$$

Continuing in this way we obtain the theorem.

From the above proof we can readily have

COROLLARY A cofactor of any infinite-dimensional matrix can be developed in terms of its principal minors:

$$A_{i_1 i_f} = -a_{i_f i_1} A^{i_1 i_f} + \sum_{m=2}^{\infty} \sum_{\substack{(i_2 i_3 \cdots i_m) \\ \neq i_1, i_f}}{}' (-1)^m a_{i_f i_2} a_{i_2 i_3} \cdots a_{i_m i_1} A^{i_1 i_2 \cdots i_m i_f} . \tag{1.6}$$

In what follows we consider Anderson model, the secular determinant of which is given by

$$|\mathbb{S}| = S = \begin{vmatrix} \ddots & & & & & & & \\ & \alpha_{-N} & -V_{-N,-N+1} & \cdots & & & & -V_{-N,N} \\ -V_{-N+1,N} & & \alpha_{N-1} & & & & & \\ & & & \ddots & & & & \\ & & & -V_{-1,0} & \alpha_0 & -V_{01} & & \\ & & & & & \ddots & & \\ & & & & & & \alpha_{N-1} & -V_{N-1,N} \\ & & & & & & -V_{N,N-1} & \alpha_N \\ & & & & & & & \ddots \end{vmatrix} \tag{1.7}$$

Here $\alpha_n = E - \varepsilon_n$, where E is energy parameter, ε_n is the energy at the nth site, and V_{nm} is the overlap integral between the nth and the m th sites. In the case of diagonally-disordered one-dimensional systems with nearest-neighbour interactions only, we have $V_{nm} = 0$ unless $|n-m| = 1, V_{n,n\pm1} = V$. Vibration of a mass-disordered linear chain with nearest-neighbour harmonic interactions only can be described also by such a secular determinant, if we put $\alpha_n = 2V - m_n \omega^2$, where now V is the spring constant of interactions and m_n is mass of the nth atom.

Applying the above theorem and corollary to the determinant S , we have

$$S = \alpha_{i_1} S^{i_1} - \sum_{m=2}^{\infty} \sum_{(i_2 i_3 \cdots i_m)}{}' V_{i_1 i_2} V_{i_2 i_3} \cdots V_{i_m i_1} S^{i_1 i_2 \cdots i_m} \tag{1.8}$$

and

$$S_{i_1 i_f} = V_{i_f i_1} S^{i_1 i_f} + \sum_{m=2}^{\infty} \sideset{}{'}\sum_{\substack{(i_2 i_3 \cdots i_m) \\ \neq i_1, i_f}} V_{i_f i_2} V_{i_2 i_3} \cdots \quad V_{i_m i_1} S^{i_1 i_2 \cdots i_m i_f} . \tag{1.9}$$

The matrix elements of Green operator of our system is, by definition,

$$\begin{aligned} G_{i_f i_1} &= (\mathcal{S}^{-1})_{i_f i_1} = S_{i_1 i_f} / S, \\ G_{i_1 i_1} &= (\mathcal{S}^{-1})_{i_1 i_1} = S^{i_1} / S . \end{aligned} \tag{1.10}$$

From the definition of the self-energy Δ_{i_1} at the i_1th site

$$G_{i_1 i_1} = \frac{1}{E - \varepsilon_{i_1} - \Delta_{i_1}} , \tag{1.11}$$

we readily obtain the relation

$$\Delta_{i_1} = \alpha_{i_1} - \frac{S}{S^{i_1}} \tag{1.12}$$

In the same way we get the general relation

$$\Delta_{i_1}^{i_2 \cdots i_m} = \alpha_{i_1} - \frac{S^{i_2 \cdots i_m}}{S^{i_1 i_2 \cdots \quad i_m}} , \tag{1.13}$$

where $\Delta_{i_1}^{i_2 \cdots \quad i_m}$ is the self-energy at the i_1th site for the system in which $\alpha_{i_2} = \alpha_{i_3} = \cdots \quad = \alpha_{i_m} = \infty$. By using (1.12) and (1.13) we have, from (1.8),

$$\begin{aligned} \Delta_{i_1} &= \sum_{m=2}^{\infty} \sideset{}{'}\sum_{(i_2 \cdots i_m)} V_{i_1 i_2} V_{i_2 i_3} \cdots \quad V_{i_m i_1} \frac{S^{i_1 i_2 \cdots i_m}}{S^{i_1}} \\ &= \sum_{m=2}^{\infty} \sideset{}{'}\sum_{(i_2 \cdots i_m)} V_{i_1 i_2} \frac{1}{\left(\dfrac{S^{i_1}}{S^{i_1 i_2}}\right)} V_{i_2 i_3} \frac{1}{\left(\dfrac{S^{i_1 i_2}}{S^{i_1 i_2 i_3}}\right)} V_{i_3 i_4} \cdots \quad V_{i_{m-1} i_m} \frac{1}{\left(\dfrac{S^{i_1 \cdots \quad i_{m-1}}}{S^{i_1 \cdots \quad i_m}}\right)} V_{i_m i_1} \\ &= \sum \sideset{}{'}\sum V_{i_1 i_2} \frac{1}{\alpha_{i_2} - \Delta_{i_2}^{i_1}} V_{i_2 i_3} \frac{1}{\alpha_{i_3} - \Delta_{i_3}^{i_1 i_2}} V_{i_3 i_4} \cdots \quad V_{i_{m-1} i_m} \frac{1}{\alpha_{i_m} - \Delta_{i_m}^{i_1 i_2 \cdots i_{m-1}}} V_{i_m i_1} . \end{aligned}$$

This is no other than Anderson's renormalized perturbation expansion (RPE) for self-energies. However, our method not only gives its very simple alternative derivation, but also shows that RPE is merely a special case of the above general mathematical theorem, which does not depend on any specific physical model. By virtue of this we can simplify many of the arguments on the analytic properties of the expansion. For example, the analytic property of the quantity $\alpha_{i_m} - \Delta_{i_m}^{i_1 i_2 \cdots i_{m-1}}$ can be seen very simply inasmuch as now it is known that this is merely the ratio $S^{i_1 \cdots i_{m-1}} / S^{i_1 \cdots i_m}$; the property of Δ_{i_1} can be discussed on the basis of the property of a single quantity $S^{i_1 i_2 \cdots i_m} / S^{i_1}$, which is a rational function with a simple structure.

In a similar way, it follows from (1.9)

$$G_{i_f i_1} = \frac{S_{i_1 i_f}}{S} = V_{i_f i_1} \frac{S^{i_1 i_f}}{S} + \sum_{m=2}^{\infty} \sum_{(i_2 \cdots i_m)}{}' V_{i_f i_2} V_{i_2 i_3} \cdots V_{i_m i_1} \frac{S^{i_1 i_2 \cdots i_m i_f}}{S}$$

$$= V_{i_f i_1} \frac{S^{i_1 i_f}}{S} + \sum_{m=2}^{\infty} \sum_{(i_2 \cdots i_m)}{}' \frac{1}{\left(\frac{S}{S^{i_f}}\right)} V_{i_f i_2} \frac{1}{\left(\frac{S^{i_f}}{S^{i_f i_2}}\right)} V_{i_2 i_3} \cdots V_{i_m i_1} \frac{1}{\left(\frac{S^{i_f i_2 \cdots i_m}}{S^{i_f i_2 \cdots i_m i_1}}\right)}$$

$$= V_{i_f i_1} \frac{S^{i_1 i_f}}{S} + \sum_{m=2}^{\infty} \sum_{(i_2 \cdots i_m)}{}' \frac{1}{\alpha_{i_f} - \Delta_{i_f}} V_{i_f i_2} \frac{1}{\alpha_{i_2} - \Delta_{i_2}^{i_f}} V_{i_2 i_3} \cdots V_{i_m i_1} \frac{1}{\alpha_{i_1} - \Delta_{i_1}^{i_f i_2 \cdots i_m}} . \tag{1.15}$$

In both of the expansions (1.14) and (1.15), each term in the expansion can be associated with a self-avoiding walk. The only difference between these two is that in the former the walk returns to the same site from which it started, while in the latter it reaches another site. Apart from this and the difference in the number of V's , these expansions have completely the same structure.

2. State-Ratio, Principal Minors of Secular Matrix and Self-Energy.

In this section we consider the special case of diagonally-disordered one-dimensional chain with nearest-neighbour interactions only. At first we briefly sketch the notion of the state ratio and its role in the problem of localization. The equation of motion of such a system is

$$-Vu_{n-1}+\alpha_n u_n - Vu_{n+1} = 0, \tag{2.1}$$

where u_n is the probability amplitude at the nth site or, in the case of vibration, the displacement of the nth atom. Equation (2.1) can be written in a vector-matrix form

$$\begin{pmatrix} u_{n-1} \\ u_n \end{pmatrix} = \begin{pmatrix} \alpha_n/V & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} u_n \\ u_{n+1} \end{pmatrix}, \tag{2.2}$$

or

$$\mathbb{X}_{n-1} = \mathbb{T}_n \mathbb{X}_n. \tag{2.3}$$

The vector $\mathbb{X}_n \equiv (u_n, u_{n+1})^T$ and the matrix $\mathbb{T}_n \equiv \begin{pmatrix} \alpha_n/V & -1 \\ 1 & 0 \end{pmatrix}$ are called state vector and transfer matrix, respectively.

If we introduce the quantity Z_n called state ratio by

$$Z_n \equiv u_{n-1}/u_n, \tag{2.4}$$

(2.1) can also be written

$$Z_n = \frac{\alpha_n}{V} - \frac{1}{Z_{n+1}} \tag{2.5}$$

If we put $t_n \equiv VZ_n$, (2.5) becomes

$$t_n = \alpha_n - \frac{V^2}{t_{n+1}}, \tag{2.6}$$

which can be written in the form of a continued fraction

$$t_n = \alpha_n - \cfrac{V^2}{\alpha_{n+1} - \cfrac{V^2}{\cdot \quad \cdot \quad \cdot}}$$

The ratio of lengths of successive state vectors is given by

$$\frac{\| x_n \|}{\| x_{n-1} \|} = \frac{(u_{n+1}^2 + u_n^2)^{1/2}}{(u_n^2 + u_{n-1}^2)^{1/2}} = \frac{1}{|z_{n+1}|} \frac{(1+z_{n+1}^2)^{1/2}}{(1+z_n^2)^{1/2}} . \tag{2.8}$$

Taking the average of lorarithm, we have

$$\left\langle \ln \frac{\| x_n \|}{\| x_{n-1} \|} \right\rangle = \left\langle \ln \frac{1}{|z_{n+1}|} \right\rangle + \left\langle \ln \frac{(1+z_{n+1}^2)^{1/2}}{(1+z_n^2)^{1/2}} \right\rangle . \tag{2.9}$$

If the distribution of Z_n is stationary, the last term will vanish, and we obtain, as a measure of average increase in the absolute amplitude of the solution of (2.1), the quantity $\bar{L}(E) = -\left\langle \ln \frac{1}{|z_{n+1}|} \right\rangle$. It has been argued that in most one-dimensional systems $\bar{L}(E)$ is positive with probability 1 [5][6][7], irrespective of the direction towards which the solution is constructed. This means that each eigenfunction is localized exponentially around a certain site which depends on the energy and the distribution of diagonal elements α_n on individual sample chain [3][4][6]. In this sense $\bar{L}(E)$ is called degree of localization.

Now, in the present case, the expansion of the self-energy (1.14) becomes simply

$$\Delta_0 = \frac{V^2}{\alpha_1 - \Delta_1^0} + \frac{V^2}{\alpha_{-1} - \Delta_{-1}^0} , \tag{2.10}$$

where

$$\Delta_{\pm 1}^0 \equiv \frac{V^2}{\alpha_{\pm 2} - \Delta_{\pm 2}^{0,\pm 1}} = \cfrac{V^2}{\alpha_{\pm 2} - \cfrac{V^2}{\alpha_{\pm 3} - \cfrac{V^2}{\alpha_{\pm 4} \cdots}}} \tag{2.11}$$

If we denote $\Delta_n^{0,1,\cdots,n-1}$ by Δ_n and put

$$S_n \equiv \begin{vmatrix} \alpha_n & -V & & \\ -V & \alpha_{n+1} & & \\ & & \ddots & \\ & & & \end{vmatrix} , \quad S_{-n} \equiv \begin{vmatrix} \ddots & & \\ & & \\ & & \alpha \quad -V \end{vmatrix} , \tag{2.12}$$

for $n \neq 0$, we have, for $n \geqq 2$,

$$\Delta_{n-1} = \frac{V^2}{\alpha_n - \Delta_n} = \cfrac{V^2}{\alpha_n - \cfrac{V^2}{\alpha_{n+1} - \cfrac{V^2}{\alpha_{n+2} \cdots}}} \tag{2.13}$$

with

$$\Delta_n = \alpha_n - \frac{S^{n-1}}{S^n} \tag{2.14}$$

From (2.13) one obtains the connection between the state ratios, principal minors and the self-energies:

$$t_n = V z_n = \frac{S_n}{S_{n+1}} = \frac{V^2}{\Delta_{n-1}} = \alpha_n - \Delta_n . \tag{2.15}$$

Thus the state ratio and the self-energy turn out to be essentially the same quantities. The degree localization can thus be expressed in terms of the self-energies:

$$L(E) = \left\langle \ln \left| \frac{V}{\Delta_{n-1}} \right| \right\rangle = \left\langle \ln \left| \frac{\alpha_n - \Delta_n}{V} \right| \right\rangle . \tag{2.16}$$

The above result strongly suggests that also in multidimensional cases, the degree of localization can be defined in terms of self-energies. In order to see how to define, let us examine the expansion (1.15) of off-diagonal elements of Green operator. In the present case this expansion becomes, for $|i_f - i_i| = p > 1$,

$$G_{i_f i_i} = V^p \frac{1}{\left(\frac{S}{S^{i_f}}\right)} \frac{1}{\left(\frac{S^{i_f}}{S^{i_f, i_f+1}}\right)} \frac{1}{\left(\frac{S^{i_f, i_f+1}}{S^{i_f, i_f+1, i_f+2}}\right)} \cdots \frac{1}{\left(\frac{S^{i_f, i_f+1, \cdots, i_i-1}}{S^{i_f, i_f+1, \cdots i_i-1, i_i}}\right)} , \tag{2.17}$$

from which we obtain

$$\frac{G_{i_f, i_i+1}}{G_{i_f, i_i}} = \frac{V}{\left(\frac{S^{i_f, i_f+1 \cdots i_i}}{S^{i_f, i_f+1 \cdots i_i, i_i+1}}\right)} = \frac{V}{\alpha_{i_i+1} - \Delta_{i_i+1}^{i_f, i_f+1 \cdots i_i}}$$

$$= \frac{V}{\cdots} = \frac{\Delta_{i_i}}{\cdots} = \frac{1}{\cdots} \tag{2.18}$$

This formula indicates that if $\overline{L}(E) = \langle \ln |z_{i_1+1}| \rangle > 0$, then the absolute value of the ratio $G_{i_f, i_1+1} / G_{i_f, i_1}$ has, on the average, a constant value less than unity; in other words, if the eigenfunction is localized, Green's function must also be localized in the sense that it decays on the average exponentially as a function of $|i_1 - i_f|$, and the exponent of average decay is given by $\overline{L}(E)$.

The above result suggests that it is reasonable to define, in multidimensional cases also, the degree of localization by the exponent of average exponential decay of Green's function. From the expansion (1.15) it is clear that $\overline{L}(E)$ must then be expressed in terms of self-energies. What should be done next is to find this expression. There has so far been no success in giving an exact expression, but in the next section it is shown that for the case of diagonally disordered systems with nearest-neighbour interactions only, $\overline{L}(E)$ can be bounded by two functions $-\ln f(E)$ and $-\ln g(E)$, which give the criterion of the convergence of RPE and the series of the first terms of the expansion of Green's function, respectively.

3. The Bounds of Degree of Localization.

In this section let us consider a diagonally disordered three-dimensional system with nearest-neighbour interactions only. To simplify the argument, we assume further that all the overlap integrals have the same value V. In this case the terms in the expansion (1.15) with $m < p \equiv |i_f - i_1|$ where $|i_f - i_1|$, the distance between the i_fth and i_1th sites, is defined as the number of steps in the shortest possible self-avoiding paths connecting these sites, vanish identically. More explicitly we have, for $p > 1$,

$$
\begin{aligned}
G_{i_f i_1} &= \sum_{m=p}^{\infty} \sum_{(i_2 \cdots i_m)}{}' V^m \frac{1}{\alpha_{i_f} - \Delta_{i_f}} \frac{1}{\alpha_{i_2} - \Delta_{i_2}^{i_f}} \cdots \frac{1}{\alpha_{i_1} - \Delta_{i_1}^{i_f i_2 \cdots i_m}} \\
&= \sum_{m=p}^{\infty} \sum_{(i_2 \cdots i_m)}{}' V^m \frac{1}{\left(\frac{S}{S^{i_f}}\right)} \frac{1}{\left(\frac{S^{i_f}}{S^{i_f i_2}}\right)} \frac{1}{\left(\frac{S^{i_f i_2}}{S^{i_f i_2 i_3}}\right)} \cdots \frac{1}{\left(\frac{S^{i_f i_2 \cdots i_m}}{S^{i_f i_2 \cdots i_m i_1}}\right)} \qquad (3.1) \\
&= \sum_{m=p}^{\infty} \sum_{(i_2 \cdots i_m)}{}' V^m \frac{S^{i_f i_2 \cdots i_m i_1}}{S}
\end{aligned}
$$

Thus what we have to do is to estimate the ratio between the series (3.1) for $|i_f - i_1| = p$ and $|i_f - i_1| = p+1$ for large p. In the one-dimensional case this was quite easy, thanks to the fact that the series consisted of a single term (2.17), but in the general case it is not an easy task. However, we can give to our series (3.1) an argument which is much the same as those of Thouless and Economou and Cohen. They discussed the convergence of RPE (1.14), and obtained the conclusion that for large m the series is bounded with very high probability by a geometric series, and there exists a function of the form

$$f(E) = VKF(E), \tag{3.2}$$

such that according as $f(E) < 1$ or > 1, RPE converges or diverges. Here K is the connectivity constant of the lattice under consideration, and $F(E)$ is a function which depends neither on V nor m. The constant K has appeared because N_s, the number of summands in the sum $\sum'_{(i_2 \cdots i_m)}$, or the number of self-avoiding walks which starts from the i_1th site and returns to the same site. It is known that K is given by $K^m m^{-7/4}$ for large m.

The precise form of the function $F(E)$ has not yet been found, apart from those which have been proposed by Thouless and Economou and Cohen on more or less physical ground. Especially the argument of Economou and Cohen involves several subtle or ambiguous points which seem to be hardly justifiable. But in any case it seems to be sure that there exists a function $f(E)$ with the form (3.2) and with the above-mentioned property, at least for a certain class of disordered systems.

Now the structure of our expansion (3.1) is quite the same as that of RPE. The only difference is that each self-avoiding walk connects the i_fth site and the i_1th site, and that the expansion starts from the term of order p. The difference in the character of self-avoiding walk does not make necessary any essential change in the argument on the convergence problem,

for it is expected that in the statistical consideration on the quantity $S_p^{i_f i_2 \cdots i_m i_i}$ the detailed shape of each individual self-avoiding walk hardly plays an important role, and also that the geometry of self-avoiding paths itself approaches that in the case of RPE as m becomes large compared with p ; the number of self-avoiding walks, for instance, evidently becomes $K^m m^{-7/4}$ for large m . Therefore it can be safely concluded that the criterion of the convergence of (3.1) is also given by the function $f(E)$.

Next we consider the series of the first terms of (3.1) for successive p- values.

By the same reason as above, for large p the argument for RPE can be applied to this series as well. We have only to replace N_s by N_f , which is the number of self-avoiding walks connecting the i_f th and i_i th sites. Actually the number N_f depends not only on the distance $p = |i_f - i_i|$ but also on the relative position of two sites. It is not difficult, however, to calculate the average number $\overline{N_s}$ for $m=p$. For example, in the case of a simple cubic lattice, it is given by

$$\overline{N_f} = \frac{2}{2p^2+1}\left\{2\sum_{i_1+i_2+i_3=p}\frac{p!}{(i_1)!(i_2)!(i_3)!} - 3\sum_{i_1+i_2=p}\frac{p!}{(i_1)!(i_2)!}\right\}$$
$$= 2^{p+1}\left\{2\times\left(\frac{3}{2}\right)^p - 3\right\}\Big/(2p^2+1). \tag{3.3}$$

For large p , this becomes $2\times 3^p/p^2$. Inasmuch as it is known that $K=4.6826$ for simple cubic lattice, we have $N_s > \overline{N_f}$, at least for sufficiently large p . Thus the series consisting of the first terms of (3.1) can be bounded with very high probability by a geometric series, the convergence of which is determined by the function

$$g(E) = VQF(E), \tag{3.4}$$

where $Q=3$ in the case of simple cubic lattice.

Now what we have to do is to compare the absolute magnitudes of $G_{i_f i_i}$ for different p-values. As explained

its convergence is determined by $f(E)$, but the terms with m which are not very much larger than p have different magnitudes from those in RPE. The difference originates from the difference between $\overline{N}_f$ and N_s. The number $\overline{N}_f$ is naturally expected to approach N_s as m becomes large. At present it is not known how $\overline{N}_f$ approaches N_s. It is reasonable, however, to assume that $\overline{N}_f$ approaches N_s monotonically, and the manner of approach does not depend on p, at least for large p. First consider the case $g(E) < f(E)$. Then the average ratio $|G_{i_f,i_1}|/|G_{i_f,i_1'}|$ which is to be put equal to $\exp(\overline{L}(E))$ is given by

$$\frac{g^p + \dfrac{f^{p+1}}{1-f}a}{g^{p+1} + \dfrac{f^{p+2}}{1-f}b} \quad \text{for } |i_f - i_1| = p,\ |i_f - i_1'| = p+1, \quad , \tag{3.5}$$

where a and b are the parameters which take the values

$$a = 1,\ b = 1. \tag{3.6}$$

if $\overline{N}_f$ becomes equal to N_s for $m \geqq p+1$, and

$$a = \left(\frac{g^{p+1}}{1-g}\right) \Big/ \left(\frac{f^{p+1}}{1-f}\right), \quad b = \left(\frac{g^{p+2}}{g}\right) \Big/ \left(\frac{f^{p+2}}{1-f}\right) \tag{3.7}$$

if $\overline{N}_f$ remains the same for all $m \geqq p$. From the assumption stated above, it follows that these parameters should have the form

$$a = (1/\alpha)^p, \quad b = (1/\alpha)^{p+1} \tag{3.8}$$

so that

$$a = b\alpha \tag{3.9}$$

where α takes the value in the interval $(1, f/g)$.
Now from the above formulas it can be shown easily

$$-\ln f(E) \leqq \overline{L}(E) \leqq -\ln g(E), \tag{3.10}$$

where the left-hand equality is valid only if $g(E)=0$ and $\alpha=1$, and the right-hand equality is valid only if $\alpha=f/g$.

In the case $g(E)>f(E)$, we have the inequality

$$-\ln f(E) > \overline{L}(E) \geqq -\ln g(E), \tag{3.11}$$

where the equality is valid only if $\alpha=f/g$ or $f=0$.

It should be emphasized here that we cannot conclude, for instance from (3.10) that the eigenfunction is not necessarily localized in Anderson's sense even when it is localized in phase-theoretical sense. The above argument leading to (3.10) is valid only if $f(E)<1$. If $f(E)>1$, then RPE diverges, and consequently the expansion of the non-diagonal elements must also diverge, irrespective of the magnitude of $g(E)$, so that there can be no localization in phase-theoretical sense also. This implies that if the eigenfunction is localized in phase-theoretical sense, then it must be localized also in Anderson's sense. Conversely, if the eigenfunction is localized in Anerson's sense, then $f(E)$ and consequently $g(E)$ must be smaller than unity, so that it must be localized also in phase-theoretical sense. Thus when $f(E)>g(E)$, the phase-theoretical concept of localization agrees with the concept of localization in Anderson's sense. The formula (3.10) indicates merely that the degree of localization is larger than $-\ln f(E)$, except in the trivial case in which $g(E)=0$ and $\alpha=1$.
If $g(E)>f(E)$, on the contrary, the eigenfunction may be non-localized in phase-theoretical sense even when it is localized in Anderson's sense. (Such a situation may arise when $f(E)<1$ but $g(E)>1$. In this case the argument leading to (3.11) is not violated.)

In connection with these points, it is interesting to remark that in the one-dimensional case we have $N_s=0$ for $m>1$ while $\bar{N}_f=1$ or 0 according as $m=p$ or $m>p$. Therefore $f(E)=0$, so that the ratio $|G_{i_f i_1}|/|G_{i_f, i_{1+1}}|$ is precisely determined by $g(E)$, which is already known to be given by $\exp\{-\langle \ln|V/\Delta_{i_1}|\rangle\}$. Thus in one-dimension the formula (3.11) is valid, though trivially. In general, however, it is quite unlikely that $\bar{N}_f$ is larger than N_s; it is even possible that the above extreme case is the only example in which $\bar{N}_f > N_s$. Especially in higher-dimensional case it is likely that we have always $\bar{N}_f < N_s$, so that what is valid is formula (3.10). Therefore it can well be expected that in most cases the two concepts of localization mentioned above agree with each other.

If the argument of Economou and Cohen is correct, the function $f(E)$ is given by their localization function $L(E)$.

4. Discussions

Our main conclusions are: (A) that it is reasonable to define the degree of localization in three-dimensional disordered systems by the exponent of average exponential decay of Green's function, and (B) that in the case of the system with nearest-neighbour interactions only, the degree of localization thus defined can be bounded by two functions $-\ln f(E)$ and $-\ln g(E)$, where $f(E)$ and $g(E)$ give the criterion of convergence of RPE and the series of the first terms of expansion of Green's function, respectively. In reaching the conclusion (B), it has been assumed (1) that RPE can be bounded asymptotically by a geometric series such that there exists the function $f(E)$ which gives the criterion for its convergence; (2) that the expansion of off-diagonal terms of Green operator can be bounded asymptotically by the same geometric series, so that the criterion of its convergence is given by $f(E)$; (3) the series of the first terms of the expansion of Green's function can be bounded by a similar geometric series, such that there exists the function $g(E)$ which gives the criterion for its convergence; (4) the number $\bar{N}_f$ approaches N_s monotonically with the increase of m. As for the assumption (1), there have been

several arguments[9)10)11)] which attempted to justify it. Although we have not yet any fully convincing justification, it seems that we can well expect that there is, at least, a class of disordered systems for which this assumption corresponds to the truth. It must be emphasized, however, that our conclusions are valid only for such systems. If we take the assumption (1) for granted, the remaining three assumptions are almost its logical consequences, though it has not yet been successfully proved with mathematical rigor. Thus, under the condition that we confine ourselves to the systems for which the first assumption can be justified, our conclusion will serve as a bridge over the gap between the phase theory and the theory of Anderson.

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REFERENCES

1) N.F. Mott and W.D. Twose, Advances in Phys. 10, 107 (1961).

2) A.P. Roberts and R.E.B. Makinson, Proc. Roy. Soc. (London) 79, 630 (1962).

3) R.E. Borland, Proc. Roy. Soc. (London) 274, 529 (1963).

4) B.I. Halperin, Adv. in Chem. Phys. 13, 123 (1967).

5) H. Matsuda and K. Ishii, Progr. Theoret. Phys. Suppl. 45, 56 (1970).

6) J. Hori, Spectral Properties of Disordered Chains and Lattices (Pergamon Press, 1968).

7) S. Minami and J. Hori, Progr. Theoret. Phys. Suppl. 45, 87 (1970).

8) B.Y. Tong, Phys. Rev. A1, 52 (1970).

9) P.W. Anderson, Phys. Rev. 109, 1492 (1958).

10) D. Thouless, J. Phys. (London) C3, 1559 (1970).

11) E.N. Economou and M.H. Cohen, unpublished.

SOLID STATE PHYSICS WORKSHOP

SOME PHASE-THEORETICAL NOTES ON LOCALIZATION OF EIGENFUNCTIONS

by

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1. A Short Summary of the Present Status

The purpose of our rather formal approach is to elucidate the nature of localization phenomenon without relying, as far as possible, on approximation which often makes the nature obscure. It is practically inevitable to stick to simple, in particular one-dimensional models, to make the theory free from approximation.

It has been known that to discuss one-dimensional models, the method of phase is particularly powerful, though in principle it can handle multidimensional systems also. In this section a short summary of the present status of phase-theoretical treatment will be given.

Let us consider at first a system which can be described by a difference equation

$$-Vu_{n-1}+\alpha_n u_n - Vu_{n+1}=0. \tag{1.1}$$

Vibration of a mass-disordered linear chain, with nearest-neighbour harmonic interactions only, is an example of the systems of this type. In this case $V=k$ is spring constant of interactions, $\alpha_n = 2k - m_n\omega^2$, where m_n is mass of the nth atom, and u_n is its displacement. Anderson's model for an electron in disordered crystal is another example, in which V is overlap integral, $\alpha_n = E-\varepsilon_n$, where ε_n is energy at the nth site, and u_n is probability amplitude at the nth site.

Equation (1.1) can be written in a vector-matrix form

$$\begin{pmatrix} u_{n-1} \\ u_n \end{pmatrix} = \begin{pmatrix} \alpha_n/V & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} u_n \\ u_{n+1} \end{pmatrix} \tag{1.2}$$

or

$$\mathbb{X}_{n-1} = \mathbb{T}_n \mathbb{X}_n. \tag{1.3}$$

We call $\mathbb{X}_n \equiv (u_n, u_{n+1})$ and $\mathbb{T}_n \equiv \begin{pmatrix} \alpha_n/V & -1 \\ 1 & 0 \end{pmatrix}$ state vector and transfer matrix respectively.

Upon introducing two linearly independent solutions u_n and v_n of (1.1), we may write

$$\begin{pmatrix} u_{n-1} & v_{n-1} \\ u_n & v_n \end{pmatrix} = \begin{pmatrix} \alpha_n/V & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} u_n & v_n \\ u_{n+1} & v_{n+1} \end{pmatrix} \tag{1.4}$$

or

$$\mathbb{U}_{m-1} = \mathbb{T}_m \mathbb{U}_m . \tag{1.5}$$

Here we choose, as u_m and v_m , the solutions which satisfy respectively the boundary conditions

$$u_N = 1,\ u_{N+1} = 0 \quad \text{and} \quad v_N = 0,\ v_{N+1} = 1. \tag{1.6}$$

Then $\mathbb{U}_N = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{I}$, so that we have

$$\mathbb{U}_{m-1} = \mathbb{T}_m \mathbb{T}_{m-1} \cdots \quad \mathbb{T}_N . \tag{1.7}$$

If we introduce the "state ratio" $z_n \equiv u_{n-1}/u_n$, (1.1) can also be written

$$z_m = \frac{\alpha_m}{V} - \frac{1}{z_{n+1}} \tag{1.8}$$

The state ratio z_n is a real quantity so far as α_n is real. We can map it onto a unit circle on the complex plane by a Cayley transform $z_m' = \frac{z_m + i}{z_m - i}$, and define its phase by $z_n' = e^{i\delta_m}$. It is important that all the quantities $\mathbb{U}_m$, z_m (or z_n') and δ_m can be calculated successively by starting from their boundary value. It will be needless to say that we may start from the other end of the system $n=0$, and proceed in the reverse direction.

In the phase theory we argue on the energy spectrum and the shape of wave functions upon the basis of the basic properties of δ_m . It is a monotonic increasing function of both n and E, and the increase of δ_0 by 2π with the increase of E means that there is one eigen-energy within this interval of E. In this way we can explain several characteristic features in the spectrum and the eigenfunctions of disordered systems, which can be described by transfer-matrix formalism (but not necessarily described by difference equation (1.1)).

In this lecture we confine our consideration on the localization of eigenfunctions.

Let $P(\delta)$ be the distribution of δ_n when we proceed in the direction of decreasing n . The phase δ_m' , which is obtained when we proceed in the reverse direction, has a distribution function $P^+(\delta)$, which is entirely different from $P(\delta)$, for

almost all values of energy parameter E . Each value of E , at which an exception occurs, gives the eigenvalue of the system under consideration. The phase δ_n changes in general slowly with E, but in the vicinity of each exceptional value of E it changes rapidly for $n \leqq n_c$, n_c being a certain value of n depending on E, and sweeps an interval whose length is nearly 2π . Likewise, δ_n' changes with energy generally only slowly; but at each exceptional energy it changes rapidly for $n \geqq n_c$. The eigenenergy is the value of E at which δ_n and δ_n' meet with each other during the rapid change of either δ_n or δ_n' or both.

Next consider the ratio of squared length of successive state vectors:

$$\frac{\|x_n\|^2}{\|x_{n-1}\|^2} = \frac{u_{n+1}^2 + u_n^2}{u_n^2 + u_{n-1}^2} = \frac{1}{z_{n+1}^2}\,\frac{1+z_{n+1}^2}{1+z_n^2} . \tag{1.9}$$

Taking the average of the logarithm, we have

$$\left\langle \ln \frac{\|x_n\|^2}{\|x_{n-1}\|^2} \right\rangle = \left\langle \ln \frac{1}{z_{n+1}^2} \right\rangle + \left\langle \ln \frac{1+z_{n+1}^2}{1+z_n^2} \right\rangle. \tag{1.10}$$

If the distribution of z_n is stationary, the last term will vanish, and we obtain, as a measure of average increase of the "intensity" of solution $\|x_n\|^2$, the quantity $\bar{L} = \left\langle \ln \frac{1}{z_{n+1}^2} \right\rangle$. It has been argued that for most one-dimensional systems $\bar{L}$ is positive with probability 1 , irrespective of the direction of transfer. This means that the eigenfunction is exponentially localized around $n = n_c$, towards both directions. In this sense $\bar{L}$ is called "degree of localization".

The theoretical arguments sketched above have been given by Roberts, Makinson, Borland, Halperin, Hori and others [1) 2) 3) 4)]. Minami and Hori[5)] confirmed the argument also numerically. Matsuda and Ishii[6)] showed that for an isotopically disordered harmonic chain $\bar{L}$ is positive with probability 1. Recently Hirota and Ishii[7)] showed that the distribution function $P(\delta)$ and consequently $\bar{L}$ can be calculated analytically for Lloyd model in which ε_n obeys Cauchy distribution.

2. State-Ratio, Principal Minors of Secular Matrix and Self-Energy.

It is an important problem to find the quantity which measures the degree of localization in multidimensional systems also, and which reduces to $\bar{L}$ in one-dimensional case. Another important problem is to elucidate the relation between our concept of localization and that of Anderson[8]. These are difficult problems and only a small step towards this direction has just begun to be made. In the following some preliminary results are reported.

It was proved by Fujita[9] that the determinant of any square matrix $|\mathbb{A}| = |\{a_{ij}\}|$ can be developed in terms of its principal minors:

$$|\mathbb{A}| = a_{i_1 i_1} A^{i_1} + \sum_{m=2}^{N} \sum_{(i_2 i_3 \cdots i_m)}{}' (-1)^{m-1} a_{i_1 i_2} a_{i_2 i_3} \cdots \; a_{i_m i_1} A^{i_1 i_2 i_3 \cdots i_m}, \quad (2.1)$$

where $A^{i_1 i_2 \cdots i_m}$ is the principal minor which is obtained by deleting from $|\mathbb{A}|$ the $i_1 th$, $i_2 th$, $\cdots$, and $i_m th$ rows and columns, and the prime means that the sum must be carried out only over all the sets of distinct indices $i_2, i_3, \cdots, i_m$. If we apply this expansion to the secular determinant of the Anderson model

$$S \equiv |E\mathbb{I} - \mathbb{H}| = \begin{vmatrix} \alpha_{-N} & -V_{-N,N+1} & \cdots & & -V_{-N,N} \\ -V_{-N+1,N} & \alpha_{N-1} & & & \\ & & & & \\ & & & \ddots & \\ & & & & \alpha_N \end{vmatrix}, \quad (2.2)$$

we obtain

$$S = \alpha_{i_1} S^{i_1} - \sum_{m=2}^{N} \sum_{(i_2, i_3, \cdots, i_m)}{}' V_{i_1 i_2} V_{i_2 i_3} \cdots \quad V_{i_m i_1} S^{i_1 i_2 \cdots i_m} \quad (2.3)$$

In the one-dimensional, diagonally disordered nearest-neighbour case, this becomes

$$S = \begin{vmatrix} \alpha_{-N} & -V & & & \\ -V & \alpha_{-N+1} & & & \\ & & \ddots \; \alpha_0 & & \\ & & & \ddots & -V \\ & & & -V & \alpha_N \end{vmatrix} = \alpha_0 S^0 - V^2 S^{0,1} - V^2 S^{0,-1} \quad (2.4)$$

or

$$\frac{S}{S^0} = \alpha_0 - \frac{V^2}{\left(\frac{S^0}{S^{0,1}}\right)} - \frac{V^2}{\left(\frac{S^0}{S^{0,-1}}\right)}. \quad (2.5)$$

If we write

$$S_\ell \equiv \begin{vmatrix} \alpha_\ell & -V & & \\ -V & \alpha_{\ell+1} & & \\ & & \ddots & \\ & & & \alpha_N \end{vmatrix} \quad \text{and} \quad S_{-\ell} \equiv \begin{vmatrix} \alpha_{-N} & -V & & \\ -V & \alpha_{-N+1} & & \\ & & \ddots & \\ & & & \alpha_{-\ell} \end{vmatrix}, \qquad (2.6)$$

then we have

$$S^0 = S_{-1} S_1, \quad S^{0,1} = S_{-1} S_2,$$

$$\frac{S^0}{S^{0,1}} = \frac{S_1}{S_2} = \alpha_1 - \frac{V^2}{\left(\frac{S_2}{S_3}\right)} = \alpha_1 - \cfrac{V^2}{\alpha_2 - \cdots - \cfrac{V^2}{\alpha_N}} . \qquad (2.7)$$

On the other hand, we obtain from (1.8), by putting $t_n \equiv V z_n$,

$$t_n = \alpha_n - \frac{V^2}{t_{n+1}} = \alpha_n - \cfrac{V^2}{\alpha_{n+1} - \cdots} \qquad (2.8)$$

Thus it turns out that successive ratios of principal minors S_n / S_{n+1} just correspond to the state ratio multiplied by V : $V z_n = S_n / S_{n+1}$.

In more general cases, in which long-range interactions are present, the expansion (2.5) becomes much more complicated:

$$\frac{S}{S^0} = \alpha_0 - \sum_{m=1}^{N} \sum_{(i_1, \cdots, i_m)}{}' V_{0 i_1} V_{i_1 i_2} \cdots \quad V_{i_m 0} \frac{S^{0 i_1 \cdots \quad i_m}}{S^0} . \qquad (2.9)$$

This may be rewritten

$$\alpha_0 - \frac{S}{S^0} = \sum_{m=1}^{N} \sum_{(i_1 \cdots i_m)}{}' V_{0 i_1} \frac{1}{\left(\frac{S^0}{S^{0,i_1}}\right)} V_{i_1 i_2} \frac{1}{\left(\frac{S^{0,i_1}}{S^{0,i_1,i_2}}\right)} V_{i_2 i_3} \cdots V_{i_{m-1} i_m} \frac{1}{\left(\frac{S^{0 i_1 \cdots i_{m-1}}}{S^{0 i_1 \cdots i_m}}\right)} V_{i_m 0} \qquad (2.10)$$

which shows that the secular determinant S can be expressed in terms of all possible ratios $S^{0, i_1, \cdots i_{m-1}} / S^{0, i_1 \cdots i_m}$.

The formula (2.10) reminds us of the renormalized perturbation expansion of the self-energy considered by Anderson[8]

$$\Delta_0(E) = \sum_{n_1}{}' V_{0 n_1} \frac{1}{\alpha_{n_1} - \Delta^0_{n_1}} V_{n_1 0} + \sum_{\substack{n_1, n_2 \\ n_1 \neq 0 \\ n_2 \neq n_1, 0}}{}' V_{0 n_1} \frac{1}{\alpha_{n_1} - \Delta^0_{n_1}} V_{n_1 n_2} \frac{1}{\alpha_{n_2} - \Delta^{0,n_1}_{n_2}} V_{n_2 0}$$

$$= \sum_{m=1}^{N} \sum_{n_1 n_2 \cdots n_m}{}' V_{0 n_1} \frac{1}{\alpha_{n_1} - \Delta^0_{n_1}} V_{n_1 n_2} \frac{1}{\alpha_{n_2} - \Delta^{0,n_1}_{n_2}} \cdots \quad V_{n_m 0} . \qquad (2.11)$$

Comparison of (2.10) and (2.11) gives identification

$$\Delta_n^{l_1 l_2 \cdots l_m} = \alpha_n - \frac{S^{l_1 l_2 \cdots l_m}}{S^{l_1 l_2 \cdots l_m; n}} . \tag{2.12}$$

Thus it turned out that the self-energies are no other than the ratio of principal minors of the secular determinant.

Since the relation (2.12) can also be obtained directly from the very definition of Green's function, Fujita's argument provides us with a very simple alternative derivation of the renormalized perturbation expansion (2.11).

In the nearest-neighbour case, (2.11) becomes

$$\Delta_0(E) = \frac{V^2}{\alpha_1 - \Delta_1^0} + \frac{V^2}{\alpha_{-1} - \Delta_{-1}^0} \tag{2.13}$$

and

$$\Delta_0^1(E) \equiv \frac{V^2}{\alpha_2 - \Delta_2^{0,1}} = \cfrac{V^2}{\alpha_2 - \cfrac{V^2}{\alpha_3 - \ddots - \cfrac{V^2}{\alpha_N}}} . \tag{2.14}$$

If we write $\Delta_m^{0,1,\cdots m-1}(E) \equiv \Delta_m$ for $m \neq 0$, we have, for $m-1 \geqq 1$,

$$\Delta_{m-1} = \frac{V^2}{\alpha_m - \Delta_m} = \cfrac{V^2}{\alpha_m - \cfrac{V^2}{\alpha_{m+1} - \ddots - \cfrac{V^2}{\alpha_N}}} \tag{2.15}$$

and

$$\Delta_m = \alpha_m - \frac{S^{m-1}}{S^m} = \alpha_m - \frac{S_m}{S_{m+1}} \tag{2.16}$$

The last formula gives the connection between the state ratio z_m and self-energy Δ_m

$$z_m = \frac{V}{\Delta_{m-1}} \tag{2.17}$$

Thus it turns out that our degree of localization is no other than the average of logarithm of squared self-energy, apart from the additive constant.

The relation (2.17) suggests that in multidimensional cases, or in the case in which long-range interactions are present, the degree of localization is given by some average over the quantities $\Delta_m^{l_1, l_2 \cdots l_m}$ or $S^{l_1 l_2 \cdots l_m}/S^{l_1 l_2 \cdots l_m; m}$. But at present it is not

yet known whether this statement is correct or not. If it is correct, it is difficult to calculate the appropriate average because these quantities cannot be obtained successively by a recurrence formula, in contrast to the one-dimensional nearest-neighbour case.

3. A Possible Measure of Degree of Localization in the Case of Long-Range Interaction.

In this section we present a method by which we can avoid the difficulty mentioned in the end of the last section. As a simple example consider the Anderson model, in which only the nearest and next-nearest interactions are present. Schrödinger's equation of this system is

$$-V'u_{n-2} - Vu_{n-1} + \alpha_n u_n - Vu_{n+1} - V'u_{n+2} = 0 \tag{3.1}$$

where $\alpha_n = E - \varepsilon_n$.

The secular matrix is

$$\mathbb{S} \equiv \begin{pmatrix} \alpha_1 & -V & -V' & & & \\ -V & \alpha_2 & -V & -V' & & \\ -V' & -V & \alpha_3 & -V & -V' & \\ & & & & \ddots & \end{pmatrix} \tag{3.2}$$

This can be partitioned as

$$\mathbb{S} = \begin{pmatrix} \mathbb{A}_1 & \mathbb{B}_2 & \\ \mathbb{B}_2^T & \mathbb{A}_2 & \\ & & \ddots \end{pmatrix} = \left(\begin{array}{cc|cc|c} \alpha_1 & -V & -V' & 0 & \\ -V & \alpha_2 & -V & -V' & \\ \hline -V' & -V & \alpha_3 & -V & \\ 0 & -V' & -V & \alpha_4 & \\ \hline & & & & \ddots \end{array}\right) \tag{3.3}$$

By putting

$$\mathfrak{u}_j = \begin{pmatrix} u_{2j-1} \\ u_{2j} \end{pmatrix}, \tag{3.4}$$

the secular equation can be written

$$\begin{pmatrix} \mathbb{A}_1 & \mathbb{B}_2 & \\ \mathbb{B}_2^T & \mathbb{A}_2 & \\ & & \ddots \end{pmatrix} \begin{pmatrix} \mathfrak{u}_1 \\ \mathfrak{u}_2 \\ \vdots \end{pmatrix} = 0, \tag{3.5}$$

which is of course equivalent to

$$\begin{pmatrix} \alpha_1 & -V & -V' & & \\ -V & \alpha_2 & -V & -V' & \\ & & & & \ddots \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \end{pmatrix} = 0 \tag{3.6}$$

The equation (3.1) may be written in a transfer-matrix form:

$$\mathbb{X}_{n-1} \equiv \begin{pmatrix} u_{n-2} \\ u_{n-1} \\ u_n \\ u_{n+1} \end{pmatrix} = \begin{pmatrix} -\frac{V}{V'} & \frac{\alpha_n}{V'} & -\frac{V}{V'} & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} u_{n-1} \\ u_n \\ u_{n+1} \\ u_{n+2} \end{pmatrix} = \mathbb{T}_n^{(0)} \mathbb{X}_n . \qquad (3.7)$$

If the system terminates at the $2Nth$ atom, we must put

$$\mathbb{X}_{2N} = \begin{pmatrix} u_{2N-1} \\ u_{2N} \\ 0 \\ 0 \end{pmatrix} . \qquad (3.8)$$

This is consistent with the form of the matrix $\mathcal{S}$. For the moment we shall assume that the system is semi-infinite in the direction of decreasing n .

Now we define the new transfer matrix by

$$\mathbb{T}_n \equiv \mathbb{T}_{2n-1}^{(0)} \mathbb{T}_{2n}^{(0)} . \qquad (3.9)$$

Then

$$\mathbb{T}_n = \begin{pmatrix} -\frac{V}{V'} & \frac{\alpha_{2n-1}}{V'} & -\frac{V}{V'} & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} -\frac{V}{V'} & \frac{\alpha_{2n}}{V'} & -\frac{V}{V'} & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} .$$

$$= \begin{pmatrix} \frac{V^2}{V'^2} + \frac{\alpha_{2n-1}}{V'} & -\frac{V}{V'^2}\alpha_{2n} - \frac{V}{V'} & \frac{V^2}{V'^2} - 1 & \frac{V}{V'} \\ -\frac{V}{V'} & \frac{\alpha_{2n}}{V'} & -\frac{V}{V'} & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} , \qquad (3.10)$$

But since

$$\mathbb{B}_n^{T} = \begin{pmatrix} -V' & -V \\ 0 & -V' \end{pmatrix}$$

$$\mathbb{B}_n^{T^{-1}} = \frac{1}{V'^2} \begin{pmatrix} -V' & V \\ 0 & -V' \end{pmatrix}$$

$$-\mathbb{B}_n^{T^{-1}} \mathbb{A}_n = -\frac{1}{V'^2} \begin{pmatrix} -V' & V \\ 0 & -V' \end{pmatrix} \begin{pmatrix} \alpha_{2n-1} & -V \\ -V & \alpha_{2n} \end{pmatrix}$$

$$= -\frac{1}{V'^2}\begin{pmatrix} -V'\alpha_{2n-1} - V^2 & VV' + V\alpha_{2n} \\ VV' & -V'\alpha_{2n} \end{pmatrix}$$

$$-\mathbb{B}_n^{T-1}\mathbb{B}_n = -\frac{1}{V'^2}\begin{pmatrix} -V' & V \\ 0 & -V' \end{pmatrix}\begin{pmatrix} -V' & 0 \\ -V & -V' \end{pmatrix}$$

$$= -\frac{1}{V'^2}\begin{pmatrix} V'^2 - V^2 & -VV' \\ VV' & V'^2 \end{pmatrix}$$

$\mathbb{T}_n$ turns out to be

$$\mathbb{T}_n = \begin{pmatrix} -\mathbb{B}_n^{T-1}\mathbb{A}_n & -\mathbb{B}_n^{T-1}\mathbb{B}_n \\ \mathbb{I} & \mathbb{O} \end{pmatrix}. \tag{3.11}$$

If we use the new transfer matrix, the equation (3.7) can be written

$$\mathbb{X}_{n-1} = \mathbb{T}_n \mathbb{X}_n,$$

where

$$\mathbb{X}_n = \begin{pmatrix} \mathcal{U}_n \\ \mathcal{U}_{n+1} \end{pmatrix} = \begin{pmatrix} u_{2n-1} \\ u_{2n} \\ u_{2n+1} \\ u_{2n+2} \end{pmatrix} = \mathbb{x}_{2n}. \tag{3.12}$$

Now we consider two independent solutions u_n and v_n , which fulfill the boundary conditions

$$\mathbb{x}_{2N} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \text{and} \quad \mathbb{x}_{2N} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \tag{3.13}$$

respectively. Then the matrix-vector

$$\mathbb{U}_n \equiv \begin{pmatrix} u_{n-1} & v_{n-1} \\ u_n & v_n \\ u_{n+1} & v_{n+1} \\ u_{n+2} & v_{n+2} \end{pmatrix} \equiv \begin{pmatrix} \mathbb{U}_n^{11} \\ \mathbb{U}_n^{21} \end{pmatrix} \tag{3.14}$$

also satisfies the equation

$$\mathbb{U}_{n-1} = \mathbb{T}_n \mathbb{U}_n, \tag{3.15}$$

with the boundary condition

$$\mathbb{U}_{2N} = \begin{pmatrix} \mathbb{I} \\ \mathbb{O} \end{pmatrix}. \tag{3.16}$$

Or if we consider other two solutions ω_n and χ_n which associate with the boundary conditions

$$\mathbb{X}_{2N} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \quad \text{and} \quad \mathbb{X}_{2N} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}, \tag{3.17}$$

then the matrix solution

$$\mathbb{U}_n = \begin{pmatrix} u_{n-1} & v_{n-1} & \omega_{n-1} & \chi_{n-1} \\ u_n & v_n & \omega_n & \chi_n \\ u_{n+1} & v_{n+1} & \omega_{n+1} & \chi_{n+1} \\ u_{n+2} & v_{n+2} & \omega_{n+2} & \chi_{n+2} \end{pmatrix} = \begin{pmatrix} \mathbb{U}_n^{11} & \mathbb{U}_n^{12} \\ \mathbb{U}_n^{21} & \mathbb{U}_n^{22} \end{pmatrix} \tag{3.18}$$

satisfies Eq.(3.15) with the boundary condition

$$\mathbb{U}_{2N} = \mathbb{I} \tag{3.19}$$

Next let us investigate the relation between the transfer matrices $\mathbb{T}_n$ and the secular matrix $\mathbb{S}$ or its determinant. Contrary to the case of the nearest-neighbour interaction, however, this becomes quite formidable unless we introduce a new concept of matrix-determinant of $\mathbb{S}$. This is defined in the same way as for the ordinary determinant by regarding each matrix entry in (3.37) as ordinary scalar matrix elements. We must of course be careful to keep the order of row-index in order to avoid the trouble which may be brought about by the non-commutability of the matrix entries. The matrix-determinant thus defined is not a scalar but a 2 x 2 matrix. Let us denote it by $\mathcal{S}$ and the ordinary determinant by $|S|$.

For the product of transfer matrices we have, for instance,

$$\mathbb{T}_{N-1}\mathbb{T}_N = \begin{pmatrix} -\mathbb{B}_{N-1}^{T^{-1}}\mathbb{A}_{N-1} & -\mathbb{B}_{N-1}^{T^{-1}}\mathbb{B}_{N-1} \\ \mathbb{I} & \mathbb{O} \end{pmatrix}\begin{pmatrix} -\mathbb{B}_N^{T^{-1}}\mathbb{A}_N & -\mathbb{B}_N^{T^{-1}}\mathbb{B}_N \\ \mathbb{I} & \mathbb{O} \end{pmatrix}$$

$$= \begin{pmatrix} \mathbb{B}_{N-1}^{T^{-1}}\mathbb{A}_{N-1}\mathbb{B}_N^{T^{-1}}\mathbb{A}_N - \mathbb{B}_{N-1}^{T^{-1}}\mathbb{B}_{N-1} & \mathbb{B}_{N-1}^{T^{-1}}\mathbb{A}_{N-1}\mathbb{B}_N^{T^{-1}}\mathbb{B}_N \\ -\mathbb{B}_N^{T^{-1}}\mathbb{A}_N & -\mathbb{B}_N^{T^{-1}}\mathbb{B}_N \end{pmatrix} \tag{3.20}$$

From now on we shall specialize in our model and put

$$\mathbb{B}_n = -\mathbb{V} = \begin{pmatrix} V' & V \\ 0 & V' \end{pmatrix}$$

Then (3.20) becomes

$$\mathbb{T}_{N-1}\mathbb{T}_N = \begin{pmatrix} \mathbb{V}^{T^{-1}}\mathbb{A}_{N-1}\mathbb{V}^{T^{-1}}\mathbb{A}_N - \mathbb{V}^{T^{-1}}\mathbb{V} & -\mathbb{V}^{T^{-1}}\mathbb{A}_{N-1}\mathbb{V}^{T^{-1}}\mathbb{V} \\ \mathbb{V}^{T^{-1}}\mathbb{A}_N & -\mathbb{V}^{T^{-1}}\mathbb{V} \end{pmatrix} \tag{3.21}$$

Next we define the matrix

$$\mathbb{S}' = \begin{pmatrix} \mathbb{V}^{T^{-1}}\mathbb{A}_1 & -\mathbb{V}^{T^{-1}}\mathbb{V} & & & & & \\ -\mathbb{V}^{T^{-1}}\mathbb{V}^T & \mathbb{V}^{T^{-1}}\mathbb{A}_2 & & & & & \\ & & \ddots & & & & \\ & & & \mathbb{V}^{T^{-1}}\mathbb{A}_{k-1} & -\mathbb{V}^{T^{-1}}\mathbb{V} & & \\ & & & -\mathbb{V}^{T^{-1}}\mathbb{V}^T & -\mathbb{V}^{T^{-1}}\mathbb{V} & & \\ & & & & & \ddots & \\ & & & & & \mathbb{V}^{T^{-1}}\mathbb{A}_{N-1} & -\mathbb{V}^{T^{-1}}\mathbb{V} \\ & & & & & -\mathbb{V}^{T^{-1}}\mathbb{V}^T & \mathbb{V}^{T^{-1}}\mathbb{A}_N \end{pmatrix}$$

and denote by $\mathbb{S}'^{i_1 \cdots i_k}$ the matrix which is obtained by deleting the i_1th, i_2th,..., and i_kth rows and columns from $\mathbb{S}'$. Now

$$\mathbb{S}'^{1,2,\cdots,N-2} = \begin{pmatrix} \mathbb{V}^{T-1}\mathbb{A}_{N-1} & -\mathbb{V}^{T-1}\mathbb{V} \\ -\mathbb{V}^{T-1}\mathbb{V}^{T} & \mathbb{V}^{T-1}\mathbb{A}_N \end{pmatrix} \tag{3.23}$$

$$\begin{aligned} S'^{1,2,\cdots N-2} &= \mathbb{V}^{T-1}\mathbb{A}_{N-1}\mathbb{V}^{T-1}\mathbb{A}_N - \mathbb{V}^{T-1}\mathbb{V}\mathbb{V}^{T-1}\mathbb{V}^{T} \\ &= \mathbb{V}^{T-1}\mathbb{A}_{N-1}\mathbb{V}^{T-1}\mathbb{A}_N - \mathbb{V}^{T-1}\mathbb{V} \end{aligned} \tag{3.24}$$

In the same way we have

$$S'^{1,2,\cdots N-2,N} = \mathbb{V}^{T-1}\mathbb{A}_{N-1}, \quad S'^{1,\cdots N-2,N-1} = \mathbb{V}^{T-1}\mathbb{A}_N . \tag{3.25}$$

If we define

$$S'^{1,\cdots N-2,N-1,N} \equiv \mathbb{I}, \tag{3.26}$$

then we find that (3.21) can be written

$$\mathbb{T}_{N-1}\mathbb{T}_N = \begin{pmatrix} S'^{1,2,\cdots N-2} & -S'^{1,\cdots N-2,N}\mathbb{V}^{T-1}\mathbb{V} \\ S'^{1,\cdots N-2,N-1} & -S'^{1,\cdots N-2,N-1,N}\mathbb{V}^{T-1}\mathbb{V} \end{pmatrix}. \tag{3.27}$$

In general we obtain the result

$$\mathbb{T}_k\mathbb{T}_{k+1}\cdots\mathbb{T}_N = \begin{pmatrix} S'^{1,\cdots,k-1} & -S'^{1,\cdots k-1,N}\mathbb{V}^{T-1}\mathbb{V} \\ S'^{1,\cdots k-1,k} & -S'^{1,\cdots k-1,k,N}\mathbb{V}^{T-1}\mathbb{V} \end{pmatrix} \tag{3.28}$$

This can be proved by induction as follows. For k = 2 it has already been proved. If

$$\mathbb{T}_{k+1} \cdots \quad \mathbb{T}_N = \begin{pmatrix} S'^{1,\dots,k} & -S'^{1,\dots k,N}\,\mathbb{V}^{T-1}\mathbb{V} \\ S'^{1,\dots k,k+1} & -S'^{1,\dots k,k+1,N}\,\mathbb{V}^{T-1}\mathbb{V} \end{pmatrix},$$

(3.29)

then

$$\mathbb{T}_k \cdots \quad \mathbb{T}_N = \mathbb{T}_k(\mathbb{T}_{k+1} \cdots \quad \mathbb{T}_N)$$

$$= \begin{pmatrix} \mathbb{V}^{T-1}\mathbb{A}_k & -\mathbb{V}^{T-1}\mathbb{V} \\ \mathbb{I} & \mathbb{O} \end{pmatrix} \begin{pmatrix} S'^{1,\dots,k} & -S'^{1,\dots k,N}\,\mathbb{V}^{T-1}\mathbb{V} \\ S'^{1,\dots k,k+1} & -S'^{1,\dots k,k+1,N}\,\mathbb{V}^{T-1}\mathbb{V} \end{pmatrix}$$

$$= \begin{pmatrix} \mathbb{V}^{T-1}\mathbb{A}_k S'^{1,\dots k} - \mathbb{V}^{T-1}\mathbb{V} S'^{1,\dots k,k+1} & \begin{matrix} -\mathbb{V}^{T-1}\mathbb{A}_k S'^{1,\dots k,N}\,\mathbb{V}^{T-1}\mathbb{V} \\ +\mathbb{V}^{T-1}\mathbb{V} S'^{1,\dots k,k+1,N}\,\mathbb{V}^{T-1}\mathbb{V} \end{matrix} \\ S'^{1,\dots k} & -S'^{1,\dots k,N}\,\mathbb{V}^{T-1}\mathbb{V} \end{pmatrix}$$

(3.30)

But since

$$S'^{1,\dots,k-1} = \mathbb{V}^{T-1}\mathbb{A}_k S'^{1,\dots k} - \mathbb{V}^{T-1}\mathbb{V}\,\mathbb{V}^{T-1}\mathbb{V}^{T} S'^{1,\dots k+1}$$

$$S'^{1,\dots k-1,N} = \mathbb{V}^{T-1}\mathbb{A}_k S'^{1,\dots k,N} - \mathbb{V}^{T-1}\mathbb{V}\,\mathbb{V}^{T-1}\mathbb{V}^{T} S'^{1,\dots k+1,N}$$

(3.31)

(3.30) just becomes (3.28). QED.

The theorem proved above gives a relation

$$\mathbb{U}_m = \mathbb{T}_{m+1} \cdots \qquad \mathbb{T}_N \mathbb{U}_N = \begin{pmatrix} S'^{1,\dots,m} \\ S'^{1,\dots m+1} \end{pmatrix}.$$

(3.32)

Thus if we define the "norm" $\|\mathbb{U}_n\|$ of the matrix-vector $\mathbb{U}_n$ by

$$\|\mathbb{U}_n\|^2 = |\mathbb{U}_n^{(11)}|^2 + |\mathbb{U}_n^{(21)}|^2, \tag{3.33}$$

then we have

$$\frac{\|\mathbb{U}_n\|^2}{\|\mathbb{U}_{n-1}\|^2} = \frac{|S'^{1,\cdots,n}|^2 + |S'^{1,\cdots\ n,n+1}|^2}{|S'^{1,\cdots n-1}|^2 + |S'^{1,\cdots\ n}|^2} \tag{3.34}$$

If we define

$$S'_{n+1} \equiv S'^{1,\cdots\ n},$$

then this becomes

$$\frac{\|\mathbb{U}_n\|^2}{\|\mathbb{U}_{n-1}\|^2} = \frac{1}{\dfrac{|S'_{n+1}|^2}{|S'_{n+2}|^2}} \; \frac{1 + \dfrac{|S'_{n+1}|^2}{|S'_{n+2}|^2}}{1 + \dfrac{|S'_n|^2}{|S'_{n+1}|^2}} \,. \tag{3.35}$$

Taking the average of logarithm, we get

$$\left\langle \ln \frac{\|\mathbb{U}_n\|^2}{\|\mathbb{U}_{n-1}\|^2} \right\rangle = \left\langle \ln \frac{|S'_{n+2}|^2}{|S'_{n+1}|^2} \right\rangle + \left\langle \ln\left\{1 + \frac{|S'_{n+1}|^2}{|S'_{n+2}|^2}\right\}\right\rangle + \left\langle \ln\left\{1 + \frac{|S'_n|^2}{|S'_{n+1}|^2}\right\}\right\rangle . \tag{3.36}$$

If it is assumed that the distribution of $|S'_{n+1}|^2/|S'_{n+2}|^2$ is stationary, the second and third terms of the r.h.s. cancel each other so that we have

$$\left\langle \ln \frac{\|\mathbb{U}_n\|^2}{\|\mathbb{U}_{n-1}\|^2} \right\rangle = \left\langle \ln |S'^{-1}_{n+1}|\,|S'_{n+2}| \right\rangle . \tag{3.37}$$

If we define the matrices $\mathbb{B}_k$ and $\mathbb{W}$ by

$$\mathbb{V}^{T-1}\mathbb{A}_k \equiv \mathbb{B}_k \qquad \text{and} \qquad \mathbb{V}^{T-1}\mathbb{V} = \mathbb{W}, \tag{3.38}$$

then the first relation in (26) becomes

$$S'_k = B_k S'_{k+1} - \mathbb{W} S'_{k+2} \tag{3.39}$$

or

$$S'_k S'^{-1}_{k+1} = \mathbb{B}_k - \mathbb{W} S'_{k+2} S'^{-1}_{k+1}$$

This is a recurrent formula for the matrix $S'_{k+2} S'^{-1}_{k+1}$, so that it can be calculated successively by starting from $S'_1 S'^{-1}_0 = \mathbb{B}_N$.

The physical meaning of the norm $\| \mathbb{U}_n \|$ is not so clear compared with the nearest-neighbour case. But this demerit may be saved at least to some extent by the following argument. In terms of the amplitudes of the solution it is

$$|\mathbb{U}_n^{(11)}|^2 + |\mathbb{U}_n^{(21)}|^2 = \begin{vmatrix} u_{n-1} & v_{n-1} \\ u_n & v_n \end{vmatrix}^2 + \begin{vmatrix} u_{n+1} & v_{n+1} \\ u_{n+2} & v_{n+2} \end{vmatrix}^2. \tag{3.40}$$

In the nearest-neighbour case the determinant $\begin{vmatrix} u_{n-1} & v_{n-1} \\ u_n & v_n \end{vmatrix}$ is just Wronskian which is to be strictly conserved. But now Wronskian is given by the determinant (3.18) so that expression (3.40) is not necessarily conserved. If the system is periodic, however, this expression can at most oscillate. Therefore if it turns out that it increases or decreases without limit, then we can safely conclude that there occurs localication.

The above method may be applied not only to the cases in which interactions of longer range are present, but also to any miltidimensional systems.

REFERENCES

1) A.P. Roberts and R.E.B. Makinson, Proc. Roy. Soc. (London) 79, 630 (1962).

2) R.E. Borland, Proc. Roy. Soc. (London) 274, 529 (1963).

3) B.I. Halperin, Adv. in Chem. Phys. 13, 123 (1967).

4) J. Hori, Spectral Properties of Disordered Chains and Lattices (Pergamon Press, 1968).

5) S. Minami and J. Hori, Progr. Theoret. Phys. Suppl. 45, 87 (1970).

6) H. Matsuda and K. Ishii, Progr. Theoret. Phys. Suppl. 45, 56 (1970).

7) T. Hirota and K. Ishii, unpublished.

8) P.W. Anderson, Phys. Rev. 109, 1492 (1958).

9) T. Fujita, unpublished.

SOLID STATE PHYSICS WORKSHOP

THEORY OF LOCALISATION IN DISORDERED SYSTEMS

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1. Introduction.

Some ten years ago an eminent Cambridge physicist said that there were no outstanding problems left in solid state physics which were sufficiently challenging to be given to the best students when they started on their post-graduate careers. I think the theory of localisation in disordered systems is one (perhaps not the only one) example that this statement is perhaps an exageration. Even now there is no formal theory of disordered systems which we can use to calc late standard properties such as conductivity, optical absorption, and Hall effect. However, the foundations of such a theory are in the process of being laid, and perhaps this branch of solid state physics will become what Ziman calls "normal science" within the next five years.

The pattern of the present lectures is that I want first (section 2) to review some experimental facts about disordered systems which given knowledge of the existence and character of the electronic states, i.e. whether they are present or not, and whether they are localised or not. This review will present certain chosen aspects and is not intended to be exhaustive.

Section 2 is a brief review of experimental evidence for the metal insulator transition in disordered systems. Section 3 deals with the failure of "traditional" G.F. approaches to the problem. Section 4 deals with a simple approach to the impurity band problem which is essential to the approach we shall use to the M.I. transitions. Section 5 introduces and discusses the Anderson model The remaining sections deal with a new approach to the M.I. transition in the three types of systems with which we are concerned.

2. We shall follow Mott in defining a state to be localised if it does not contribute to the static electrical conductivity. Let us review briefly some experimental facts about crystalline systems and their theoretical explanation.

The conductivity of a normal metal at the absolute zero of temperature is found to be infinite. For other crystalline systems the conductivity is found to be zero. These differences were explained on the Wilson-Sommerfeld model in terms of the one electron branch structure which arises from the solution of the Schrödinger equation. According to this, the wave functions in allowed regions have the form

$$\psi(\underset{\sim}{r}) = e^{i\underset{\sim}{k}.\underset{\sim}{r}} u_{n\underset{\sim}{k}}(\underset{\sim}{r}) \qquad 2\cdot1$$

in "allowed" regions which are separated from each other by forbidden regions where no bounded solutions exist. The difference between metals and insulators is then explained by the position of the Fermi level: in metals it lies in an allowed region, in insulators it lies in a gap. It can easily be shown that if the Fermi level lies in an allowed region the conductivity is infinite. This result follows either from linear response theory or from arguments which show that $\underset{\sim}{k}$ increases indefinitely on application of a field. In the insulator the Fermi level is in a gap, and the Valence band is full and the conduction band empty. It is therefore a sufficient condition for the conductivity to be zero for the density of states to be zero at the Fermi level. It is essential to understand that this is a sufficient and not a necessary condition.

Insulators exist whose existence is not explained in the one-electron theory (e.g. NiO). At least in some cases this can be explained on the basis of a many body argument due to Mott and Hubbard. Essentially the argument is that in a band Coulomb interactions can split the band so that a Fermi level which would lie in a band on one-electron theory in fact lies in a gap. The correct electron spectrum having been found, the distinction between metals and insulators follows as before.

If the gap between valence and conduction bank is sufficiently small thermal excitation can create an appreciable number of electrons in the conduction bank and holes in the valence band. In this case simple theory shows that the conductivity has the form:

$$\sigma = \sigma_0 \exp - E_g/2kT \qquad 2.2$$

This relation is experimentally confirmed and provides a method for determining E_g. A plot of log σ v T^{-1} has the form show in Fig. 1.

Conversely an experimental result of this form is interpreted as implying the existence of an activation energy, i.e. of an energy gap.

Optical absorption also measures the energy necessary to excite an electron from the valence band to the conduction band. For parabolic bands and direct transitions the absorption coefficient has the approximate form:

$$\alpha(\omega) = C(\omega-\omega_0)^{1/2} \qquad 2.3$$

where

$$\hbar\omega_0 = E_g \qquad 2.4$$

Experimental results of the form of Fig. 2 again are interpreted as implying the existence of a gap in the spectrum of electron states.

We now turn to experimental results on disordered systems. Here I wish to consider three types: 1) systems which give rise to impurity bands; 2) highly doped semiconductors; 3) amorphous semiconductors.

Some impurities, when put into a semiconductor in low concentration, produce additional states in the gap (e.g. Sb in Ge). These states can be seen, e.g. in optical absorption, as sharp lines. It is also possible to see transitions between two impurities as shown in luminescence.

As the density of donors is increased the luminescent line shape changes from a line to a Gaussian type curve (Fig. 3). On a simple argument this shape is proportional to the density of states and such results are therefore interpreted as showing that impurity - impurity interactions broaden the line into a continuous curve. As the density of impurities increases, the the experiments suggest that the density of states merges with the conduction band. With very high doping the absorption curve eventually looks like Fig. 4.

Comparison with Fig. 2 suggests that there is now a continuous distribution of states below the conduction band. Normally the experimental results are fitted by a curve of the form:

$$\alpha(\omega) = A \exp -\left(\frac{E}{E_0}\right)^{\alpha} \qquad 2.5$$

The absorption curve of most amorphous materials also has the same form, $\lambda \to 1$ being the most common value. The density of states is now continuous with the conduction band and has a similar form shown in Fig. 5.

All the evidence suggests that when a semiconductor has a low density of impurities, the Fermi level is in the impurity band It is therefore surprising that where the density of impurities falls below a certain value, the conductivity falls by several orders of magnitude to a value which is experimentally indistinguishable from zero. The concentration when this happens is of the order of 3-4 effective Bohr radii. Since the conductivity is found to be zero in the impurity band, although luminescence measurements show that there are states at the Fermi level, we are found to conclude that there are certain states which can contribute to optical properties but which give zero conductivity. We call these localised states. Fig. 6 gives the experimental results for the conductivity as a function of T^{-1}. which also illustrate this transition. As the concentration increases the activation energy is seen to increase and eventually to go to zero. Fig. 7 gives further results for the conductivity for experiments in which acceptors are also present.

Experiments have also been carried out with much higher concentrations, e.g. for Na in Argon and Cu in Argon. The concentration at which the transition takes place is much higher, corresponding to about 15% and 40% respectively. The density of states is then presumably of the form shown in Fig. 5. There is no reason to believe that the Fermi level is in a region where the density of states is zero.

In the case of amorphous semiconductors, the conductivity has typically the temperature dependence shown in Fig. 8, showing the existence of a well defined activation energy. On the other hand, the absorption coefficient behaves as shown in Fig. 9. This again presents apparent contradictions: the presence of an activation energy shows that these are states which do not contribute to the conductivity, whereas the absorption coefficient data suggest a continuous distribution of states. The contradiction was resolved by the Mott-Cohen theory of a mobility gap which is illustrated in Fig. 10.

The experiments which we have described are typical of those which support the idea that there are electronic states present which do not contribute to the conductivity. In the next section we shall consider the "traditional" Green's function approach to such problems and why it fails.

3. <u>The failure of "traditional" theories of disordered systems.</u>

What we describe as the traditional theory of disordered systems is summarised in "Lectures on the Mathematical Theory of Disordered Systems", to which we shall refer.

In the traditional theory we study the behaviour of the average G.F., e.g. in $\underset{\sim}{k}$ representation, which may be written

$$\langle\langle G^{+}(\underset{\sim}{k})\rangle\rangle = \frac{1}{E - k^{2} - \Sigma(\underset{\sim}{k}, E)} \qquad 3.1$$

Now linear response theory enables us to write the conductivity as

$$\sigma \sim \mathrm{Tr}\left[v\,(\mathrm{Im}\, G^{+})\, v\,(\mathrm{Im}\, G^{+}) \right] \qquad 3.2$$

Here $\langle\langle\ \ \rangle\rangle$ denotes an average in a statistical sense over whatever cause of disorder is present, e.g. impurity positions (cf. L.M.T.D.S).

Suppose that for the moment we assume $\langle\langle g\, v\, g\rangle\rangle = \langle\langle g\rangle\rangle\, v \langle\langle g\rangle\rangle$ where

$$g = \mathrm{Im}(G^{+}) \qquad 3.3$$

Then put $$\Sigma(k, E) = A + iB \tag{3.4}$$

3.5

It can be shown on general grounds that $B \geq 0$. If $B \neq 0$ then 3.2 has the form

$$\sigma \sim \int \frac{k^2 B^2 \, d^3k}{[(E - k^2 - A)^2 + B^2]^2} \tag{3.6}$$

which is clearly non zero if $B \neq 0$ and $\to \infty$ as $B \to \infty$
It is therefore difficult to see how, from such a theory, a result of the form

$$\sigma = 0 \quad . \tag{3.7}$$

$$N(E) = -\pi^{-1} \operatorname{Tr} \operatorname{Im}(G^+) \tag{3.8}$$

could emerge. It is not difficult to find more detailed contradictions. Thus, consider how we could try to describe an impurity band by approximation 4 of L.M.T.D.S. (p. 26). Essentially here $\Sigma(k, E) = \rho\, t(k, k)$. A look at the details in the one dimensional case shows that while an impurity band is formed Σ is purely real within the band, implying infinite life time and therefore conductivity. Again, all approximations for Σ in the one dimensional case lead to $\operatorname{Im} \Sigma = 0$ at some finite E , for all concentrations, in contradiction to the exponential behaviour which would be expected from the absorption data for high densities.

These shortcomings are, I believe, essentially due to the fact that the k representation is not a good one for the problem. A localised state implied local asymmetry; the k representation implies translational invariance. This symmetry must be broken if localised states are to be obtained.

4. The density of states in an impurity band.

In order to obtain a feel for the problem, let us consider the impurity band case first; the understanding of this is essential to enable a correct theory to be formulated, as has been emphasized by Mott.

A defect of the mormal self energy expansions considered in L.T.D.S. is that it does not provide a form of self energy which reduces to the correct atomic limit in the low density case. In the atomic limit we can write the G.F.

$$G^+(\underset{\sim}{r},\underset{\sim}{r}',E) = \sum_n \frac{\psi_n(\underset{\sim}{r})\,\psi_n(\underset{\sim}{r}')}{E-E_n} \qquad 4.1$$

where the $\psi_n(\underset{\sim}{r})$ are the atomic wave functions. For E_n near a particular E_n, say E_0, we can write

$$G^+(\underset{\sim}{r},\underset{\sim}{r}',E) \doteq \frac{\psi_0(\underset{\sim}{r})\,\psi_0(\underset{\sim}{r}')}{E-E_0+i\varepsilon} \qquad 4.2$$

which gives $\quad \operatorname{Im} G^+(\underset{\sim}{r},\underset{\sim}{r}') = -i\pi\,\psi_0(\underset{\sim}{r})\psi_0(\underset{\sim}{r}')\,\delta(E-E_0) \qquad 4.3$

then we get $\quad -\pi^{-1}\,\mathrm{Tr}\left[\operatorname{Im} G^+(\underset{\sim}{r},\underset{\sim}{r},E)\right] = \delta(E-E_0) \qquad 4.4$

which is intuitively correct.

Now consider the corrections due to this as a result of a low density of impurities, so that an electron can see several impurities. By analogy with the virial expansion we can consider interactions between pairs only in first approximation. Defining the propagator $K(t)$ by

$$\int_0^\infty e^{iEt}\,K(t)\,dt = i\,G^+(E) \qquad 4.5$$

we obtain using the approximation 4.2

$$K(\underset{\sim}{r},\underset{\sim}{r}',t) = \psi_0(\underset{\sim}{r})\,\psi_0(\underset{\sim}{r}')\,e^{-iE_0t} \qquad 4.6$$

and for an atom at site α $\quad K_0(\underset{\sim}{r},\underset{\sim}{r}',t) = \psi_0(\underset{\sim}{r}-\underset{\sim}{t}_\alpha)\,\psi_0(\underset{\sim}{r}'-\underset{\sim}{t}_\alpha)\,e^{-iE_0t} \qquad 4.7$

we now write $$H = H_0 + H_I \tag{4.8}$$

where $$H_0 = p^2/2m + v(r - R_\alpha) \tag{4.9}$$

$$H_I = v(r - R_\beta) \tag{4.10}$$

$$K(r, r', t) = \langle r | e^{-i(H_0 + H_I)t} | r' \rangle \tag{4.11}$$

4.11 can be expanded in the usual way

$$K(r, r', t) = K_0(r, r', t) + \int_0^t K_0(r, r'', \tau) H_I(r'') K_0(r'', r', t-\tau) \, dr'' d\tau + \cdots \tag{4.12}$$

If we took just the first term this would correspond to the Born approximation which would not be adequate as we are interested in a perturbation which changes the poles of 4.2 and must therefore sum an infinite series of terms, in some sense or other. The simplest procedure is to be a cumulant approxiamation (Lukes, Somaratna, and Tharmalingam, 1970).

Essentially we write

$$K(r, r', t) = K_0(r, r', t) \exp \sum_{n=1}^{\infty} \frac{k_n}{n!} (-i)^n \tag{4.13}$$

where for example

$$k_1 = \int_0^t K_0(r, r'', \tau) H_I(r'') K_0(r'', r', t-\tau) \, d\tau \, dr'' \Big/ K_0(r, r', t-\tau) \tag{4.14}$$

Using 4.10 and 4.6 we obtain

$$k_1 = t \int \psi_0(r - R_\alpha) v(r - R_\beta) \psi_0(r - R_\alpha) \, dr \tag{4.15}$$

If we take the $\psi_0(\underline{r})$ to be an s state this can be written

$$h_1 = t F |\underline{R}_\alpha - \underline{R}_\beta| \tag{4.16}$$

We now use 4.5 to obtain

$$G(\underline{r}, \underline{r}', E) = \frac{\psi_0(\underline{r}-\underline{R}_\alpha)\,\psi_0(\underline{r}-\underline{R}_\alpha)}{E - E_0 - F(R)} \tag{4.17}$$

This expression must now be average over both $\underline{R}_\alpha - \underline{R}_\beta$ and over $\underline{R}_\alpha$.
i.e. we sum over all pairs of atoms.
For N impurities in a volume (see L.T.D.S.)

the average over the α is

$$\sum_\alpha \psi_0(\underline{r}-\underline{R}_\alpha)\,\psi_0(\underline{r}-\underline{R}_\alpha)\,\frac{d\underline{R}_\alpha}{\Omega} = \sum_\alpha \frac{1}{\Omega} = \frac{N}{\Omega} = \rho \tag{4.18}$$

where ρ is the number density of impurities.

We now average over the distances $\underline{R} = |\underline{R}_\alpha - \underline{R}_\beta|$. For a random distribution the distribution of nearest neighbours is a Hertz distribution:

$$p(R) = 4\pi R^2 \rho \; \exp -\tfrac{4}{3}\pi R^3 \rho \tag{4.19}$$

The average density of states can then be written

$$\begin{aligned} N(E) &= -\pi^{-1}\, \mathrm{Tr} \langle\langle \operatorname{Im} G^+(\underline{r}, \underline{r}, E) \rangle\rangle \\ &= \int_\Omega d\underline{r}\, \rho\, \delta[E - E_0 - F(R)]\, p(R)\, dR \\ &= \Omega \rho \sum_i \frac{\exp -\left(\frac{4}{3}\pi R_i^3 \rho\right) 4\pi R_i^2 \rho}{\left|\frac{dF}{dR}\right|_{R=R_i}} \end{aligned} \tag{4.20}$$

where the sum is taken over all values of R which satisfy

$$E - E_0 + F(R) = 0 \tag{4.21}$$

For a known $\psi_0(r)$ the integral over 4.20 can be carried out of necessary numerically. This has been done taking for $\psi_0(r)$ hydrogenic ground state wavefunctions. Near $E-E_0$ the result can be expressed analytically:

$$n(E) = \frac{4\pi\zeta}{C} \left[\frac{C}{E-E_0}\right]^4 \exp -\frac{4}{3}\pi\zeta \left(\frac{C}{E-E_0}\right)^3 \qquad 4.22$$

where $n(E)$ is the density of states per atom. For $\zeta \to 0$ this reduces to $\delta(E-E_0)$ [equation 4.4] as it should. The result looks like Fig. 11 . Fig. 12 shows a typical result of a more complicated calculation carried out by the same sort of method where we have included the effect of both donors and acceptors and also, in a simple way, electron correlation [Lukes, Somaratna and Agrell, unpublished]. At least in this approximation the Coulomb interaction splits the band, but I shall not consider the effect of electron correlations in any detail in these lectures. These results could (and perhaps should) be extended to include higher order cumulants.

5. The Anderson model for the insulator metal transitions.

Having obtained a reasonable model for the density of states in an impurity band we now discuss the question of whether these states are localised or not. A great step forward in attacking such problems was taken by Anderson (1958). We shall refer to his discussion as the Anderson model (not to be confused with the Anderson Hamiltonian).

In the context of the results we have discussed, Anderson's argument may be expressed as follows. The result 4.16 shows that the energy levels ε are modified by a fluctuating term $F(R)$. Therefore instead of considering a distribution of distances in 4.16 we could write

$$F(R) = \varepsilon \qquad 5.1$$

$$p(R)\,dR = \rho(\varepsilon)\frac{dR}{d\varepsilon}\,d\varepsilon \qquad 5.2$$

We could now write 4.17

$$G^+(\underline{r},\underline{r}',E) = \frac{\psi_0(\underline{r}-\underline{R}_\alpha)\,\psi_0(\underline{r}'-\underline{R}_\alpha)}{E-E_0-\varepsilon} \qquad 5.3$$

where the ε have a probability distribution.

The problem we have been considering is complicated by the fact that the $\underline{R}_\alpha$ have a random distribution. An essential part of Anderson's contribution was to recognise that this was really irrelevant to the problem. Anderson in fact put his atoms in a periodic lattice. This enables him to introduce Wannier functions which are labelled by the sites α,β; in fact his model is defined by the Hamiltonian

$$H_{\alpha\beta} = \varepsilon_\alpha \delta_{\alpha\beta} \qquad \alpha = \beta \qquad 5.4$$

$$H_{\alpha\beta} = V \qquad \alpha,\beta \quad \text{nearest neighbours.} \qquad 5.5$$

We shall only consider a simple cubic lattice here. Here V is taken to be a constant independent of α,β ; it can be taken to be analogous to $F(R)$ for a periodic lattice.

In terms of these

we can write down the equation for the G.F. as

$$G = G_0 + G_0 H_I G \qquad 5.6$$

where $$\langle\alpha|G_0|\beta\rangle = \frac{1}{E-\varepsilon}\delta_{\alpha\beta} \qquad 5.7$$

Expanding 4.24 iteratively we get

$$\langle\alpha|G|\beta\rangle = \frac{1}{E-\varepsilon_\alpha}\delta_{\alpha\beta} + \frac{1}{E-\varepsilon_\alpha} V_{\alpha\gamma} \frac{1}{E-\varepsilon_\gamma} \qquad 5.8$$

where we have temporarily labelled the V's by the lattice sites which they connect but shall, in fact, take them all to be the same. The ε's in 4.26 are now defined with respect to E_0 .

From the shape of the density of states we can guess that a rectangular density of states would not be a bad approximation. We keep the height of the distribution the same and fix the width W by the normalisation condition.

Using 4.22 we get for example

$$N(E_{max}) = \bar{R} \exp -\frac{4}{3}\pi^{-4/3}(0.554)^{-1} \qquad 5.9$$

where $\bar{R}$ is the mean distance between the impurities which is related to the density by

$$\bar{R} = 0.554\,\rho^{-1/3} \qquad 5.10$$

hence we define $$W = N(E_{max})^{-1} \qquad 5.11$$

For the moment, we can now forget about the random positions of the impurities and study the model Hamiltonian defined by 4.22 and 4.23, with the proviso that the ϵ's are independently distributed of one another with distribution

$$p(\epsilon) = W^{-1} \qquad -\frac{W}{2} < \epsilon < \frac{W}{2} \qquad 5.12$$

For a long time the relationship of the Anderson model to the random impurity problem was badly understood. It was Mott who, in a series of papers, recognised the major importance of Anderson's work and that it could form the basis of a new approach to the metal-insulator transition in a number of apparently different cases.

Anderson's argument was now essentially as follows. In a time dependent representation the proper factor corresponding to 5.7 is

$$\langle \alpha | u(t) | \beta \rangle = e^{-i\epsilon_\alpha t}\,\delta_{\alpha\beta}. \qquad 5.13$$

and corresponds to an electron localised at site α. If the electron is to diffuse away from the site, this localised state must decay. Now, using the standard G.F. methods we can sum 5.6

into an expression by means of the self energy. If we do so we would expect 5.13 to have a factor

$$e^{-i(\varepsilon-\Sigma)t} = e^{-i[\varepsilon-A-iB]t}$$

Hence we must have $B>0$ for the state to decay. Hence the condition for the electron to diffuse away is for the imaginary part of the self energy to be non zero. Now if one writes down an expression for the self energy, curiously enough the first few terms are real. A simple example of this occurs in our expression 4.16 in which $F(A)$ can be interpreted as a term in Σ. Thus it appears that the state never decays! Anderson's argument now was to examine the convergence of the series for Σ. This was found to be determined by the ratio V/W, and Anderson argued that the value of V/W at which the series diverged could be interpreted as that at which an electron begins to diffuse away from the state. Thus we have a model of an insulator-metal transition in the one-electron approximation. Mott has suggested that this model can in fact be used to explain metal insulator transitions in all the cases we have considered, using semi-quantitative arguments.

A review of Anderson's work has been given by Thouless (1970) and comments have been made by Ziman (1970). Nevertheless, Anderson's theory is not very suited to practical applications. The connection of his argument with the observed phenomenon, electrical conductivity, is very formal, nor can his work be directly applied to the three types of system we have in mind. In the following sections I want to describe a different approach which attempts to remedy these deficiencies.

6. The Conductivity in the Anderson Model.

In contrast to the usual situation in the theory of disordered systems, it is the unperturbed G.F. which is subject to a probability distribution and we define average G.F.

$$g_0 = \langle\langle G_0 \rangle\rangle \tag{6.1}$$

$$g = \langle\langle G \rangle\rangle \tag{6.2}$$

where the bracket $\langle\langle \; \rangle\rangle$ now denotes an average over the ε_i.

In the Wannier representation Dyson's equation becomes a matrix equation :

$$\underset{\sim}{G} = \underset{\sim}{G_0} + \underset{\sim}{G_0}\,\underset{\sim}{H_I}\,\underset{\sim}{G} = \underset{\sim}{G_0} + \underset{\sim}{G_0}\,\underset{\sim}{H_I}\,\underset{\sim}{G_0} \qquad 6.3$$

with solution $\underset{\sim}{G} = \left[\underset{\sim}{G_0}^{-1} - \underset{\sim}{H_I}\right]^{-1}$ 6.4

From 6.3 we can define a self-energy Σ by

$$g = g_0 + g_0 \Sigma g \qquad 6.5$$

$$\Sigma = g_0^{-1} - g^{-1} \qquad 6.6$$

The equation for the static electrical conductivity can be written in the form (we use units such that $\hbar = 1$)

$$\sigma_{\mu\nu} = \lim_{\omega \to 0} e^2 \omega^2 \pi^2 \int \frac{\partial f}{\partial E}\, dE\, \mathrm{Tr}\left\{ \delta(E_F - H)\, r_\mu\, \delta(E_F + \hbar\omega - H)\, r_\nu \right\} \qquad 6.7$$

Hence f is the Fermi function.

Specialising to the case of zero temperature and putting

$$\delta(E - H) = -(2\pi i)^{-1}\left[G^+(E) - G^-(E)\right] \qquad 6.8$$

6.7 can be written

$$\sigma_{\mu\nu} = \lim_{\omega \to 0} \frac{\omega^2}{\pi}\, \mathrm{Real}\; \mathrm{Tr}\left[r_\mu \left\{ G^+(E)\, r_\nu\, G^+(E + \hbar\omega) - G^+(E)\, r_\nu\, G^-(E + \hbar\omega) \right\}\right] \qquad 6.9$$

For the Anderson Model we need to write this in terms of Wannier functions. In order to do so, we use the result

$$\langle i | r | j \rangle = r_i \delta_{ij}$$

Here i, j label sites. Equation 6.9 can now be written

$$\sigma_{\mu\nu} = \lim_{\omega \to 0} \frac{\omega^2}{\pi}\, \mathrm{Real}\Big[\Big\langle\!\Big\langle \sum_{ij} r_i^{\mu}\, G_{ij}^{+}(E_F)\, r_j^{\nu}\, G_{ji}(E_F + \hbar\omega) - r_i^{\mu}\, G_{ij}^{+}\, r_j^{\nu}\, G_{ji}^{-}(E + \hbar\omega)\Big]\qquad 6.10$$

We define

$$\Pi_\nu = \langle\langle G^{\alpha} \gamma_\nu G^{\beta} \rangle\rangle \qquad 6.11$$

It is seen that the contribution to the conductivity must be of order ω^{-2} in order that a finite conductivity is obtained. In the present case no such factor occurs. Thus the conductivity goes to zero as ω^{2}. We can also use this argument to show, e.g. that for a single electron in an atomic state the conductivity is zero. We shall therefore agree that the condition for a finite value of conductivity is that the series for Π_ν will diverge. Since the separate terms of the series are finite up to $\omega \to 0$ we shall take this limit in the summand of 6.10 from now on.

7. The integral equation for Π_ν.

If $F(z)$ denotes the power series

$$F(z) = c_0 + c_1 z + c_2 z^2 + \cdots$$

Then the Cauchy-Hadamard method of determining the ratios of convergence depends on the series $|c_1|, |c_2|^{1/2} \ldots |c_n|^{1/n}$. If the greater limit of the sequence is by then $r = \ell^{-1}$.

$$\langle\langle G \rangle\rangle = \frac{1}{g^{-1} + G_0^{-1} - (H_I + g^{-1})} = \frac{1}{g^{-1} - A} \qquad 7.1$$

where
$$A = H_I + g^{-1} - G_0^{-1} \qquad 7.2$$

Thus
$$G = g + gAG \qquad 7.3$$

putting this into 6.11 and considering $\alpha = \beta = +$ for simplicity we obtain

$$\Pi_\nu = \langle\langle g + gAG \rangle\rangle \gamma_\nu (g + gAG) \rangle\rangle$$
$$= g\gamma_\nu g + \langle\langle gAG\gamma_\nu g \rangle\rangle + \langle\langle g\gamma_\nu GAg \rangle\rangle$$
$$+ \langle\langle gAG\gamma_\nu GAg \rangle\rangle$$

7.4

This equation is, so far, exact. We now consider the second term

$$\begin{aligned} \langle\langle\, g\, A\, G\, \gamma_\nu\, g \,\rangle\rangle &= g \langle\langle A\, G \rangle\rangle\, \gamma_\nu\, g \\ &= g \langle\langle \left[G_0^{-1} - G^{-1} + g^{-1} - G_0^{-1} \right] G\, \gamma_\nu\, g \rangle\rangle \\ &= 0 \end{aligned} \qquad 7.5$$

The third term is similarly found to be zero.

The last term is

$$\langle\langle\, g \left[H_E + g^{-1} - G_0^{-1} \right] G\, \gamma_\nu\, G \left[H_E + g^{-1} - G_0^{-1} \right] g$$

$$\sim g \left(H_E - \Sigma \right) \Pi_\nu \left(H_E - \Sigma \right)$$

We now obtain

$$\Pi_\nu = g\, \gamma_\nu\, g + g \left(H_E - \Sigma \right) \Pi_\nu \left(H_E - \Sigma \right) \qquad 7.6$$

an equation of the Bethe-Salpeter type for Π_ν . This leads to the iterative expansion

$$\begin{aligned} \Pi_\nu = {} & g\, \gamma_\nu\, g + g \left(H_E - \Sigma \right) g\, \gamma_\nu\, g \left(H_E - \Sigma \right) g \\ & + g \left(H_E - \Sigma \right) g \left(H_E - \Sigma \right) \gamma_\nu\, g \left(H_E - \Sigma \right) g \left(H_E - \Sigma \right) g \\ & + \cdots \end{aligned}$$

8. <u>Divergence of the Bethe- Salpeter Eq^{n}.</u>

In order to study the divergence of the series for Π_ν we meat an exact expression for g which is difficult to obtain.

However, we can obtain an upper bound to the value of V/W by replacing g by g_0 in 7.7 , i.e. we put

$$\langle \alpha |\, g\, | \beta \rangle \sim g_0 = \langle\langle \frac{1}{E - \varepsilon} \rangle\rangle\, \delta_{\alpha\beta} \qquad 8.1$$

Using the distribution 5.12 we get

$$g_0 = W^{-1} \ln \left[\frac{E + i\varepsilon + W/2}{E + i\varepsilon - W/2} \right] \qquad 8.2$$

To estimate Σ we consider the approximation of a self-avoiding walk. Asymptotically the number of terms is K^n for both the diagonal and off diagonal terms, where K is the connectivity constant of the lattice.

Hence we obtain for the n^{th} term $g_0 V^{N-1} K^N$ and for the sum

$$g_{\lambda\mu} = \frac{1}{g_0^{-1} - VK} \tag{8.3}$$

Hence in this approximation the diagonal and off diagonal elements of the G.F. are the same and given by

$$\Sigma = VK \tag{8.4}$$

Putting 7.11 and 7.9 into 7.7, we again consider a self avoiding walk approximation. In this case the series 7.7 is geometric and the condition for the series to diverge is

$$g_0^2 |(V - \Sigma)|^2 K^2 \geqslant 1 \tag{8.5}$$

We now consider the centre of the band and put $E = 0$ in 8.2 This leads to a critical value of $W/V = 54$ which is in fact an upper bound to this value.

Using methods which I do not have time to discuss, we can also estimate the lower bound to be about 25.4. The upper bound is, in fact, fairly close to the estimate obtained by Anderson.

9. The impurity band problem.

We now consider the impurity band problem which forms an important part of the evidence for the Anderson transition.

In order to apply the method of the previous sections, we need to consider the G.F. for this model, which can be obtained from the Dyson expansion

$$G(\underline{r}, \underline{r}', E) = \sum_\lambda \frac{\psi_0(\underline{r} - \underline{R}_\lambda)\psi_0(\underline{r}' - \underline{R}_\lambda)}{E - E_0}$$
$$+ \sum_\lambda \frac{\psi_0(\underline{r} - \underline{R}_\lambda)\psi_0(\underline{r}'' - \underline{R}_\lambda)}{E - E_0} \sum_\beta v(\underline{r}'' - \underline{R}_\beta) \sum_\gamma \frac{\psi_0(\underline{r}'' - \underline{R}_\gamma)\psi_0(\underline{r}' - \underline{R}_\gamma)}{E - E_0} \tag{9.1}$$

where it is understood that the diagonal element $\lambda = \beta = \gamma ..$ is omitted since it gives rise to the atomic G.F. The remaining terms now consist of overlap integrals which may be classified into two types, namely those of the first type

and those of the second type

$$v_2(\underline{R}_\alpha - \underline{R}_\beta) = \int \psi_0(\underline{r}'' - \underline{R}_\alpha)\, v(\underline{r}'' - \underline{R}_\beta)\, \psi_0(\underline{r}'' - \underline{R}_\alpha)\, d\underline{r}'' \qquad 9.3$$

We now redefine the zero order G.F., by including in it all terms of the first type. This may be done by the cumulant procedure described in section 4. The result is that the G.F. redefined in this way is now

$$G(\underline{r}, \underline{r}', E) = \frac{\langle\langle \psi_0(\underline{r} - \underline{R}_\alpha)\, \psi_0(\underline{r}' - \underline{R}_\alpha) \rangle\rangle}{E - E_0 - F(R)} \qquad 9.4$$

where $R = |\underline{R}_\alpha - \underline{R}_\beta|$ and the brackets denote an average over both the intersite distances and over the sites α themselves. The advantage of carrying out such a partial summation is that we can now put the theory into a similar form to that previously considered for the Anderson problem. The distribution of can be replaced by a distribution of energies with a parameter defined by 5.11.

Again we obtain the Bethe-Salpeter equation as previously

$$\Pi_\gamma = q\, r_\gamma\, q + q\,(K_E - \Sigma)\,\Pi_\gamma\,(K_E - \Sigma) \qquad 9.5$$

where the only difference between these equations and those of the Anderson model is that the averages are now carried out over the random positions of the atoms and only implicitly over the energy levels.

The terms of 9.5 now involve factors of the form

$$\frac{\langle\langle \psi_0(\underline{r} - \underline{R}_\alpha)\, \psi_0(\underline{r}'' - \underline{R}_\alpha) \rangle\rangle}{E - \epsilon_1} \left[\sum_\alpha v(\underline{r}'' - \underline{R}_\alpha) - z\, v(R_{max}) \right] \frac{\langle\langle \psi_0(\underline{r}'' - \underline{R}_\beta)\, \psi_0(\underline{r}'' - \underline{R}_\beta) \rangle\rangle}{E - \epsilon_2} \qquad 9.6$$

where we have evaluated the averages over intersite distances at the maximum of the Hertz distribution which, to our order of accuracy is indistinguishable from the mean. The value of Σ is easily found to be

$$\Sigma = z\, v(R_{max}) \qquad 9.7$$

Hence we obtain for the condition 8.5

$$\left(\frac{\pi}{W}\right)^2 |\eta-1|^2 v(R_{max})^2 \geq 1 \qquad 9.8$$

Substituting a value of $\eta \sim 10$ and 5.11, 5.9 into 9.8, we obtain for the upper limit of concentration

$$\bar{R} = 3.9\ Ka \qquad 9.9$$

Where K is the dielectric constant and a the Bohr radius. We have used hydrogenic S state wave functions

$$v(R_{max}) = -2E_0\left[1+\frac{R_{max}}{a}\right] \exp - R_{max}/a \qquad 9.10$$

Using methods which I do not have time to discuss, we can show that a lower limit of the concentration is given by approximately

$$\bar{R} = 5.3\ Ka \qquad 9.11$$

10. A more general form of the localisation condition.

For the case of an impurity band, a more general and perhaps more useful form of the upper bound for V/W can be obtained. Making use of the Dirac relation

$$\frac{1}{E-\epsilon+i\epsilon} = \frac{P}{E-\epsilon} - i\pi\delta(E-\epsilon) \qquad 10.1$$

$$\mathrm{Im}\left[E-\epsilon-i\epsilon'\right] = -\pi N(E) \qquad 10.2$$

where $N(E)$ is the density of states per atom. The real part of 10.1 is given by the dispersion relation

$$\left\langle\left\langle \frac{P}{E-\epsilon} \right\rangle\right\rangle = \int \frac{N(E')\,dE'}{E-E'} \qquad 10.3$$

The form of this for a typical band has been discussed (Izyumov, 1965). It is antisymmetric about the maximum and zero there. Thus for energies near the maximum we can write

$$\left\langle\!\left\langle \frac{1}{E-\varepsilon+i\eta} \right\rangle\!\right\rangle \sim -\pi N(E) \qquad 10.4$$

and hence the condition 9.8 can be written

$$\pi(z-1)\, N(E)\, V(R_{max}) > 1 \qquad 10.5$$

This relation shows that a low density of states is favourable for localisation and exhibits clearly the existence, in general, of mobility edges in impurity bands.

11. Localisation in highly doped and amorphous semiconductors.

Experimental evidence suggests that in both highly doped and amorphous semiconductors the density of states is a montonically decreasing function of energy as we move away from the band edge of the pure material. Therefore the theory of the preceding sections cannot be directly applied to these materials. We shall, however, suggest that it can be applied in a modified form.

It is characteristic of both highly doped and amorphous materials that the random potentials are much more densely distributed than in systems which give rise to impurity bands. For such systems it is reasonable to assume that the potential at a point has a multivariate Gaussian distribution

$$p[V(\mathbf{r})] = A \exp -\frac{1}{2}\int d\mathbf{r}\, d\mathbf{r}'\, V(\mathbf{r})\, K(\mathbf{r},\mathbf{r}')\, V(\mathbf{r}') \qquad 11.1\ (a)$$

where the kernel $K(\mathbf{r},\mathbf{r}')$ can be defined in terms of the correlation function $w(\mathbf{r},\mathbf{r}')$ of the potential by the equations

$$w(\mathbf{r},\mathbf{r}') = \langle V(\mathbf{r})\, V(\mathbf{r}') \rangle \qquad 11.1\ (b)$$

$$\int d\mathbf{r}'\, K(\mathbf{r},\mathbf{r}'')\, w(\mathbf{r}'',\mathbf{r}')\, d\mathbf{r}'' = \delta(\mathbf{r}-\mathbf{r}') \qquad 11.1\ (c)$$

In systems containing a low density of impurities, natural centres of localisation exist in the impurity atoms themselves. In a highly doped material, however, the density of electrons is sufficiently great to screen out atomic bound states and the same is presumably true of amorphous semiconductors. In any case, the density of atoms is so high that it is meaningless to associate an electron with a particular atom.

A theory of localisation which applies generally to a random collection of atoms of high density has been given by Zittartz and Langer (1966) (Z.L.) and by Halperin and Lax (1966) (H.L.) Although the existence of localised states is demonstrated, no discussion is given of how the transition to non-localised states takes place. It is this particular point with which we are here concerned.

The Z – L and H – L theories put forward the idea of a non-zero average local field which is sufficiently strong to localise an electron. The effective potential acting on one electron in weak binding theories can be identified with the self energy. Because it is averaged over the free particle Green function, such an effective potential is spatially homogenous and cannot bind an electron. By assuming the existence of localised states it can be shown that an average potential can be derived which depends on the Green's function. It is given by

$$V_{eff}(\underset{\sim}{r}) = -\int d\underset{\sim}{r}''\, w(\underset{\sim}{r},\underset{\sim}{r}'')\, \frac{G(\underset{\sim}{r},\underset{\sim}{r}'')\,G(\underset{\sim}{r}'',\underset{\sim}{r}')}{G(\underset{\sim}{r},\underset{\sim}{r}')} \qquad 11.2$$

Under certain simplifying assumptions this reduces to

$$V_{eff}(\underset{\sim}{r}) = -\int d\underset{\sim}{r}'\, w(\underset{\sim}{r}-\underset{\sim}{r}')\, \psi^2(\underset{\sim}{r}')\, d\underset{\sim}{r}' \qquad 11.3$$

where the wavefunction $\psi_0(\underset{\sim}{r})$ is given by a Hartree type non-linear differential equation

$$-\frac{1}{2}\nabla^2\psi_0(\underset{\sim}{r}) - \frac{1}{E_0-E}\int d\underset{\sim}{r}'\, w(\underset{\sim}{r},\underset{\sim}{r}')\, \psi^2(\underset{\sim}{r}')\, \psi_0(\underset{\sim}{r}) = E_0\psi_0(\underset{\sim}{r}) \qquad 11.4$$

Although these equations assume that the distribution of potential can be described by the second moments alone, the theory could, in principle, be extended by including higher order correlations.

The assumption of localised states can be regarded as a symmetry condition which produces a non-zero mean field, given by 11.2, which can localise the electron.

Deep in the tail the potential given by 11.2 can be taken to be randomly distributed throughout the material with little overlap. Each potential then gives rise to a delta function in the density of states. The density of states nevertheless remains a continuous function of energy because the potentials themselves depend on energy through 11.2. As the density of states increases, the number of solutions of 1.4 in a given energy range per unit volume increases proportionately and therefore there will be increasing overlap of wavefunctions.

We can now discuss the localisation in similar terms to those which have been used to discuss impurity bands. It is convenient to refer to the centres of localisation with which we associate the potentials 11.2 as quasi atoms; with each quasi atom, we associate a quasi atom wavefunction given by 11.4. We can now define an overlap integral of quasi potentials between quasi atom wavefunctions similar to the $\psi_o(\underline{r})$ discussed in §4 . By considering the conductivity deep in the tail, we obtain a value of zero, because the Green functions used in evaluating 6.7 are of the form 4.2 where the $\psi_o(\underline{r})$ are now given by 11.4. Again, we look for a divergence in the series for the conductivity. By applying precisely the same reasoning as before we can recapture all the results of §10 . Assuming that the width W association with each energy is sufficiently small, both the bounds given previously are now close together and are given by

$$(z-1)\, e v(L_{max})\, N(E) \geq 1 \qquad 11.5\ (a)$$

$$(z-1)\, n v(L_{max})\, N(E) \geq 1 \qquad 11.5\ (b)$$

where $N(E)$ is now the average number of nearest neighbour quasi atom solutions and $N(E)$ is the density of states per quasi atom This equation again predicts the existence of mobility edges in

References. Anderson, P.W., (1958), Phys. Rev. 109, 1492.
The classical paper on the subject of localisation.
Other discussions of this are:

Brouers, F., (1970), J. Non Cryst. Solids 4, 428.

Lloyd, P., (1969), J. Phys. C., 2, 1717.

Ziman, J.M., (1969), J. Phys. C., 2, 1230. See also papers I and III by Ziman in the same series.

Thouless, D., (1970), J. Phys. C., 3, 1559.

Halperin, B.I., and Lax, M., (1966), Phys. Rev. 148, 722.

Izyumov, I., (1965), Advances in Physics 14, 569.

Mott, N.F., (1970), Phil. Mag. 22, 1. This paper contains references to the earlier papers by Mott on the subject of disordered systems. This body of work during the last ten years is a remarkable attempt to provide a unified theory of disordered systems based on the Anderson model.

Zittartz, J. and Langer, J.S., (1966), Phys. Rev. 148, 741.

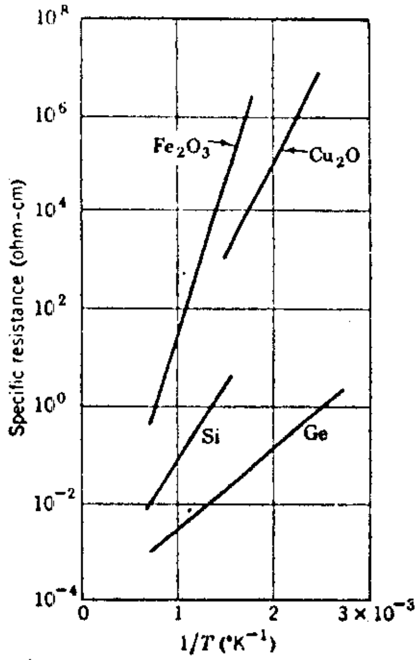

Fig. 13.3. Plot of log ρ vs. $1/T$ for several semiconductors in the intrinsic range. (After J. A. Becker.)

Fig. 1 Typical plot of log conductivity in the intrinsic region for several semiconductors in the intrinsic range [after Becker].

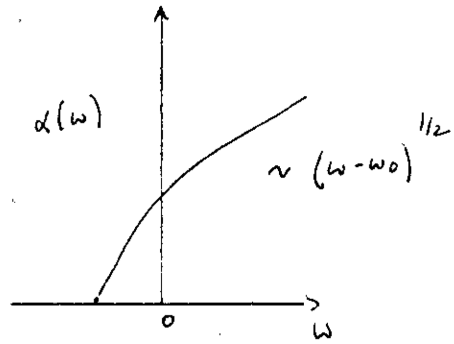

Fig. 2 Typical shape of absorption coefficient at the fundamental edge for direct transitions.

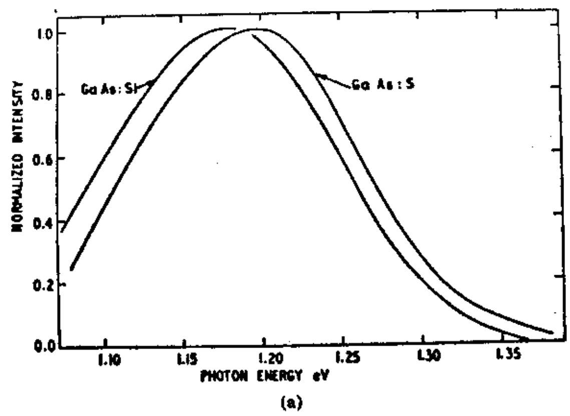

Fig. 3 Typical lineshapes observed in luminescence.

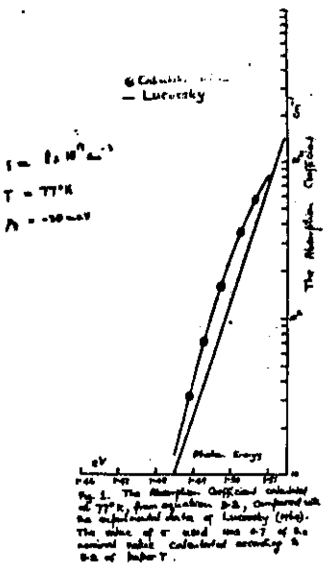

Fig. 4 Typical experimental absorption curve of a highly doped semi-conductor (.). The continuous curve is that calculated by Lukes and Somaratna [1970, J. Phys. C., 3, 2044].

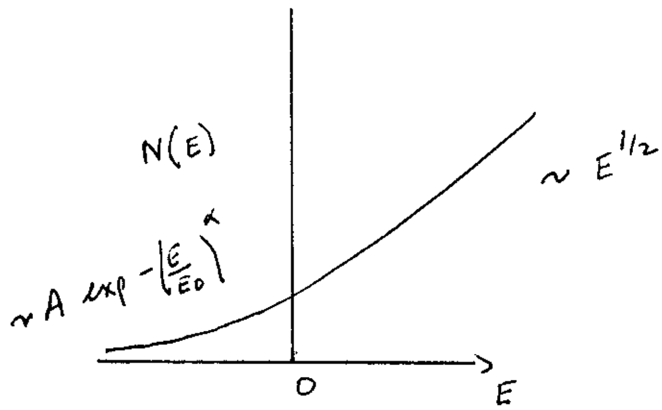

Fig. 5 Conjectured density of states curve in a highly doped semi-conductor.

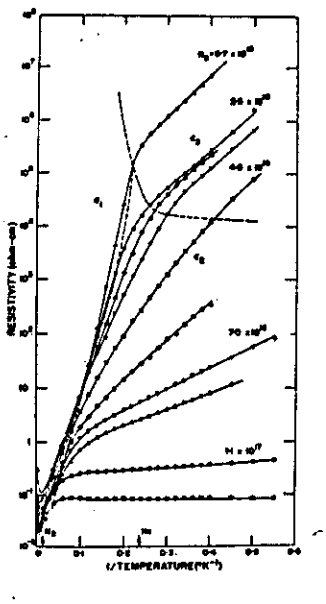

Fig. 6 Resistivity ~ T^{-1} for impurity band conduction in Sb doped Ge . Note the way in which, as the concentration is increased, the curves level off [after Davis, E.A.,

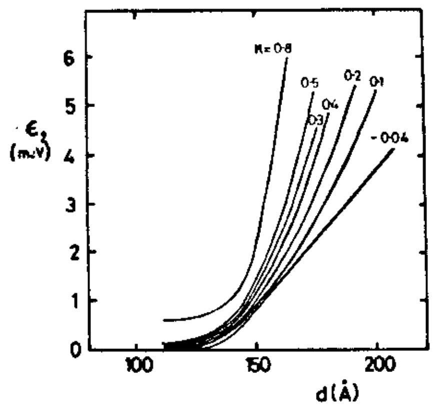

Fig. 7 Variation of activation energy, as a function of impurity separation and compensation [after Mott & Davis, 1968, Phil. Mag., 17, 1269].

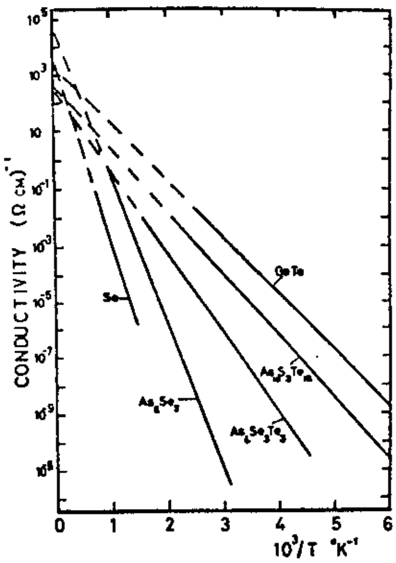

Fig. 8 Typical temperature dependence curves of conductivity in some amorphous semiconductors [after Davis, unpublished].

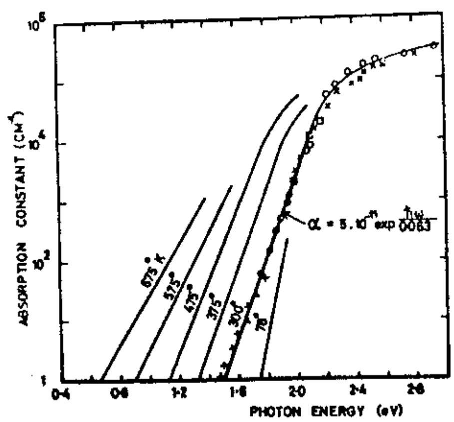

Fig. 9 Absorption coefficient of at different temperatures showing existence of a tail [after Davis, unpublished].

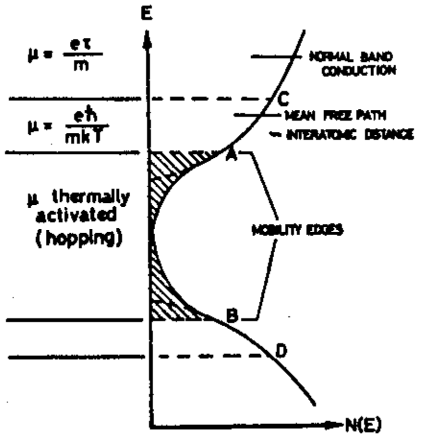

Fig. 10 Mott–Cohen theory of mobility gap.

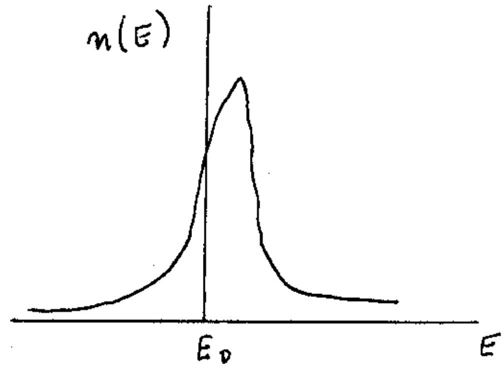

Fig. 11 Density of states due to donor–donor interaction [after Lukes, Somaratna and Tharmalingam, 1970, J. Phys. C., 12, 1631].

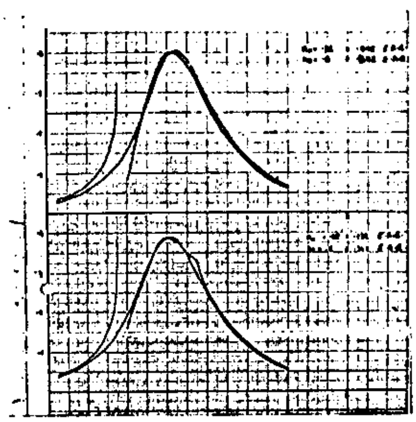

Fig. 12 Density of states in an impurity band in the presence of compensation and electron correlation [Lukes, Somaratna and Agrell, unpublished].

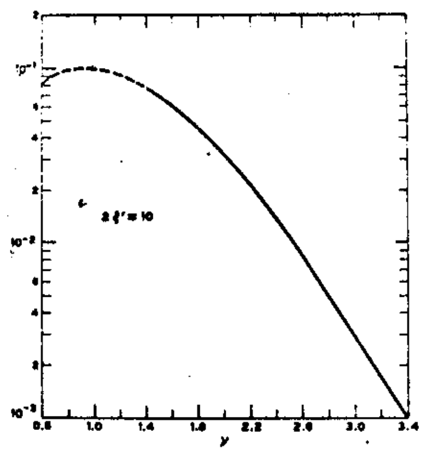

Fig. 13 Typical result for density states against energy in the theory of Halperin and Lax.

SOLID STATE PHYSICS WORKSHOP

(Short) summary of three lectures on

POLARONS

by

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INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

TRIESTE, JULY 1971.

(Short) Summary of three lectures on

POLARONS. (I.C.T.P. Trieste July 1971)

J. Devreese, Univ. Antwerp.

① Optical properties of polarons (WEAK V STRONG COUPLING).

1. Weak coupling [REF 1] [REF 2]

The optical absorption is calculated following [ref 2].

We start from the golden rule for the transition probability for a polaron to go from the groundstate to a scattering state:

a phonon is emitted
no lattice relaxation

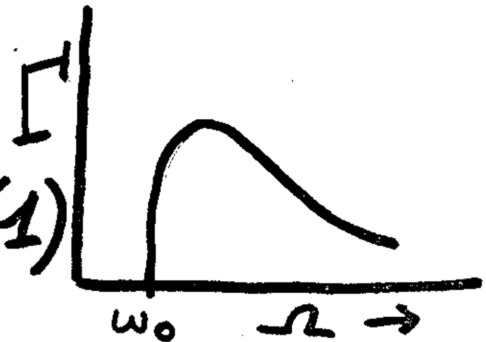
By eliminating intermediate states one obtains the KUBO-FORMULA but for T=0 and one polaron.

Subsequently the Lee Low Pines formalism is used. This formalism is based on two canonical

transformations. The first introduces the electron as "reference point." (One moves with the electron) The second takes the lattice deformation into account at weak coupling.

We obtain:

$$\Gamma = \frac{1}{c\epsilon_0 n}\,\frac{2}{3}\,\alpha\,\sqrt{\frac{\Omega-\omega_0}{\Omega^3}} \quad (1)$$



Γ = optical absorption coëfficient
Ω = frequency of the incident light.
ω_0 = long wavelength optical phonon frequency.
α = coupling constant

The derivation given in REF 2 is simple but the result (1) is a special case of results obtained in [ref 1] with highly involved techniques.

It is possible to improve eq (1) so that it is reliable for $\alpha \approx 1$
We obtain:

$$\Gamma = \frac{1}{c\epsilon_0 n}\,\frac{2}{3}\left(\frac{m^*}{m}\right)^{3/2}\alpha\,\frac{\sqrt{\Omega-\omega_0}}{\Omega^3}\,e^{-\gamma_\alpha \frac{m^*}{m}|\Omega-\omega_0|} \quad (2)$$

γ_α is a slowly varying function of α ($0.1 < \gamma < 1$).

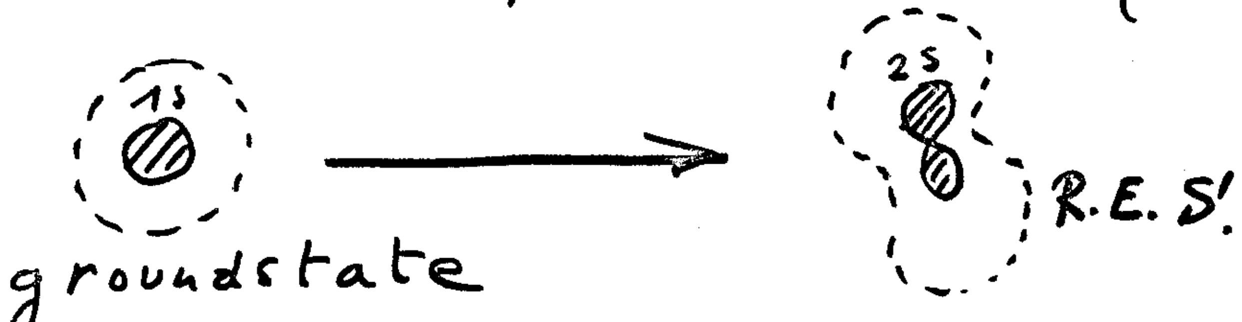
(2) is a limiting case obtained from expressions discussed below

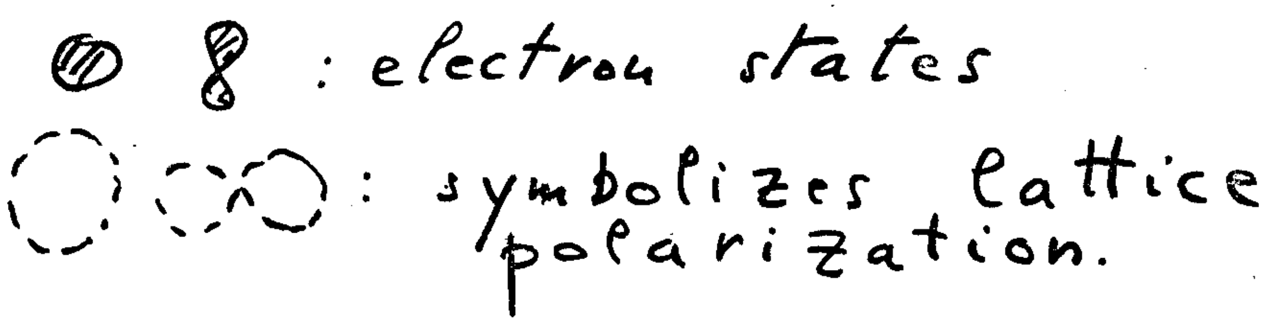
2. Strong coupling. [ref 3][ref 4]

[ref 3] is the main paper; [ref 4] contains mathematical refinements.

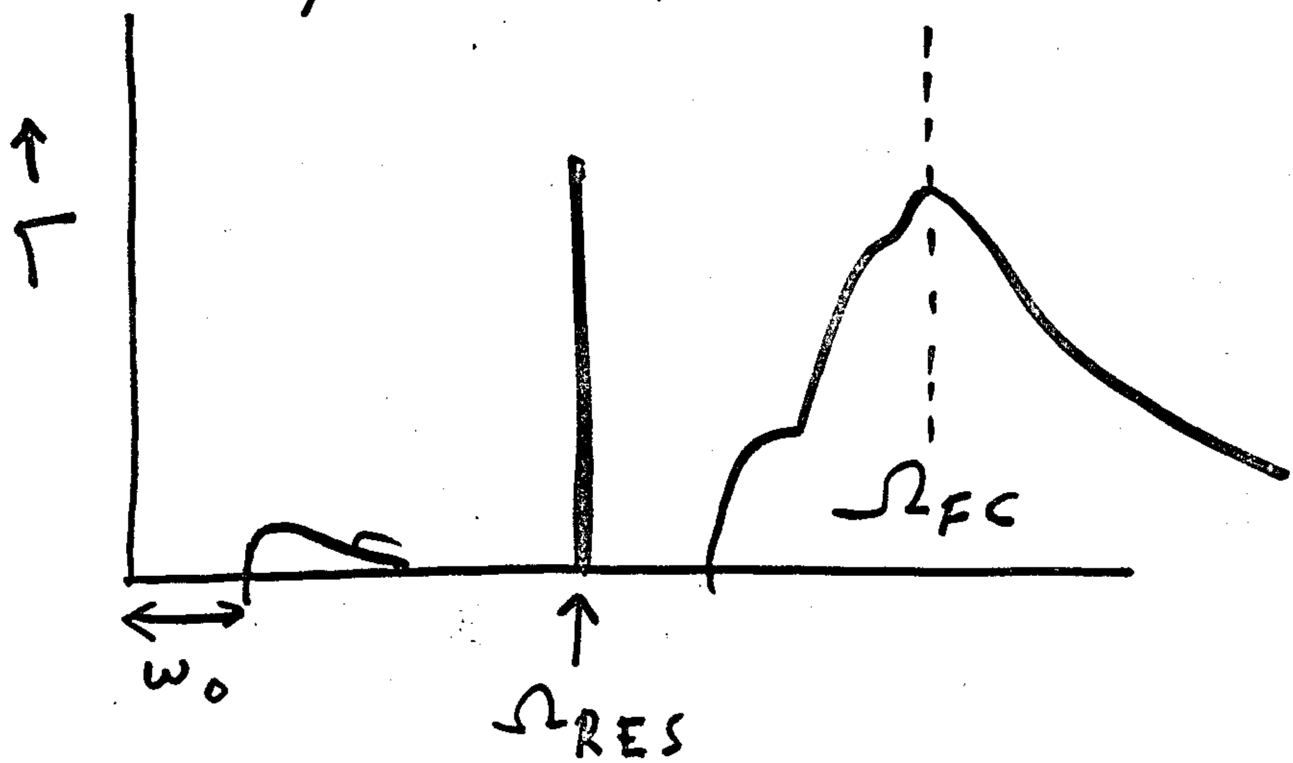
It is argued that <u>internal excitations</u> of polarons play a role at large α. LATTICE RELAXATION can occur for excited states and then one speaks of RELAXED EXCITED STATES: R.E.S.

Pictural representation: (large $\underline{\alpha}$)





With golden rule transition probability from groundstate to R.E.S.
R.E.S. + n phonons
should be calculated.
The lifetime of the R.E.S. is calculated using Wigner-Weiskopf theory.
This leads for $\alpha > 6$ to intense peak for ZERO-PHONON TRANSITION and complex SIDEBAND STRUCTURE with maximum at the "FRANCK-CONDON" frequency (no lattice readaptation)



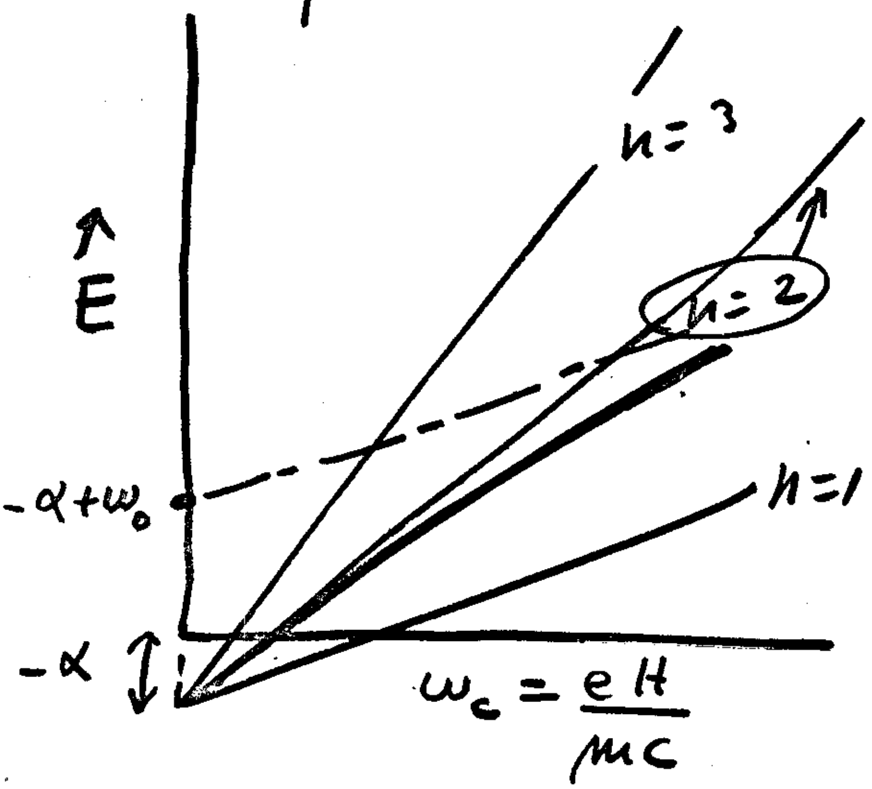
Experiment: Until now only weak coupling behaviour (eq 1) seems to have been observed [REF 5]

(2) POLARONS in MAGNETIC FIELDS [REF 6, 7]

ELECTRON–PHONON interaction modifies the Landau levels and <u>adds</u> extra levels.

1) Weak coupling (REF 6)

The spectrum becomes:



→ The $n=2$ level is "pinned" by the scattering state at $\underline{-\alpha+\omega_0}$.

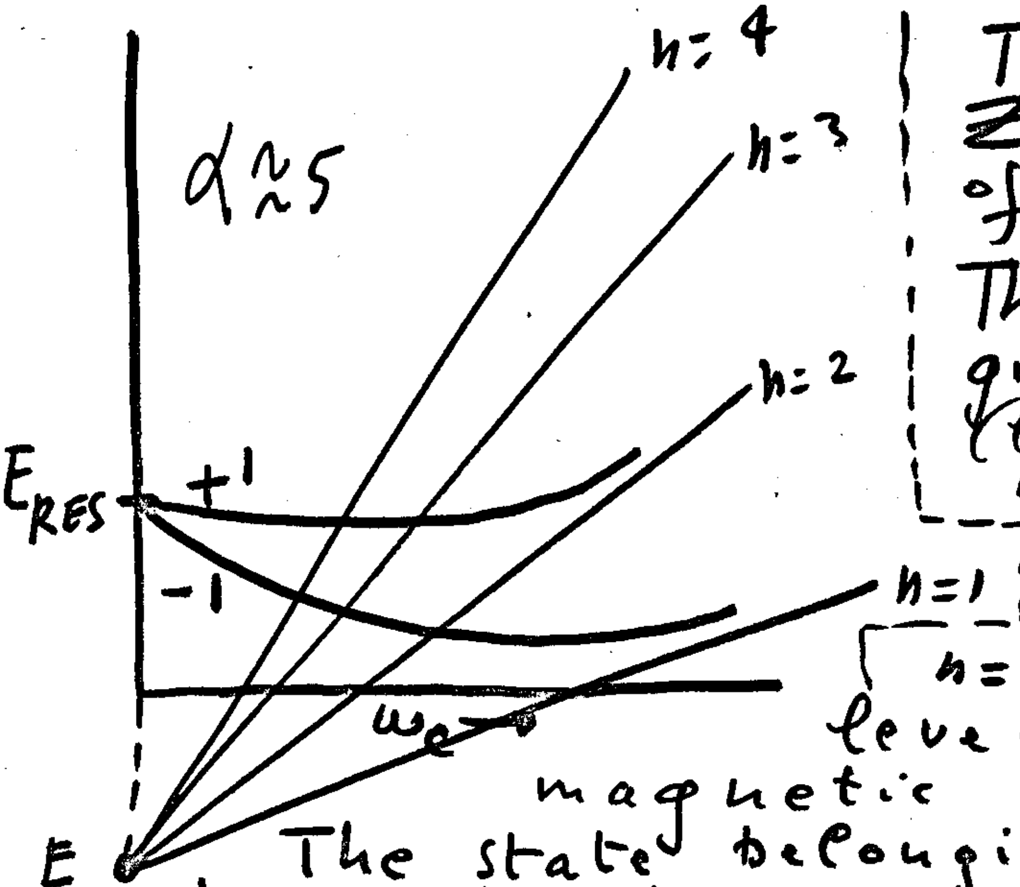
→ The slope of the LANDAU LEVELS is determined by the <u>polaron mass</u>, instead of the bare mass. Brown's [7] measurements are based on this fact. LARSEN, LAX et al. [8] have studied the <u>pinning</u>.

Also R.E.S. modify the LANDAU LEVEL SCHEME.

LEE LOW PINES

In L.L.P. approximation for z-direction ‖ and Product-Ansatz for wave functions ($\Psi = |\text{field}\rangle \varphi_{electr.}$)

we obtain:



There is a Zeeman splitting of RES.

The state belonging to $l_z = +1$ (l_z = angular momentum of the electron) tends to the n=2 Landau level for large magnetic field.

The state belonging to $l_z = -1$ tends to the n=1 Landau level for $H \to \infty$.

Recent calculations have shown that the $l_z = +1$ state gets <u>stabilized</u> if the field increases.

Therefore: HIGH MAGNETIC FIELDS ARE A TOOL TO OBSERVE R.E.S. (PRESUMABLY ONLY IF $\alpha \gtrsim 3$)

EXPER. EVIDENCE: KOBAYASHI (REF 9) observed stabilization of

③ INTERMEDIATE COUPLING; PATH INTEGRALS.

A short survey of path integral techniques is given. [see 9]

Advantages:
- No operators involved.
- One can rely on classical intuition
- phonons can be exactly eliminated (transformation of many body problem to one-particle problem)
- path integrals might even be calculated by computer.

Disadvantages:
- Until now spin could not be treated.
- Involved mathem.

One can treat exactly with path-integrals:

a) Harmonic oscillator (1948)

b) now progress: Coulomb potential ref 10, 11, 12.

The only existing intermediate [13]
coupling theory is due to Feynman,
F.H.I.P. [14], Feynman Thornber [15].

It is based on a quadratic
approximation.
after the elimination of the
phonons one concentrates on
the motion of one particle.

One supposes that the electron
moves in a quadratic potential.

FHIP calculated:

$$\frac{1}{Z(\Omega)} = \Omega\, G(\Omega)$$

$Z(\Omega)$ = impedance function

harmonic approximation:

$$\frac{1}{Z(\Omega)} = \Omega\, G_0(\Omega)$$

then they go one order further:

$$\frac{1}{Z(\Omega)} = \Omega\,(G_0 + G_1)$$

G_1 is a ~~linear~~ function of $S - S_0$:
the difference between exact and
trial action.

FHIP then consider:

$$Z(\Omega) = \frac{1}{\Omega G(\Omega)} \approx \frac{1}{\Omega(G_0+G_1)} \qquad (3)$$

and the "development"

$$Z(\Omega) = \frac{1}{\Omega}\left(\frac{1}{G_0} - \frac{G_1}{G_0^2}\right) \qquad (4)$$

They have no real justification for (4).

From (4) they obtain $\lim_{\Omega \to 0} Z(\Omega) = \frac{1}{\mu}$ (μ = the mobility) and they also plot $\mathrm{Re}\, Z(\Omega)$. $\mathrm{Re}\, Z(\Omega)$ shows structure at FRANCK-CONDON STATES.

It seems, that no lattice relaxation is taken into account.

We calculated [16]

$$\Gamma \sim \mathrm{Re}\, \frac{1}{Z(\Omega)} = \mathrm{Re}\, \frac{\Omega}{\frac{1}{G_0} - \frac{G_1}{G_0^2}} \qquad (5)$$

This leads to cumbersome analytical and numerical work.

References.

1. Gurevich et al: Sov. Phys. Sol. St., 4, 918 (1962).

2. Devreese, Huybrechts, Lemmens: Phys. Stat. Sol. (1971) (to be published).

3. E. Kartheuser, R. Evrard, J. Devreese: Phys. Rev. Letters, 22, 94 (1969).

4. M. Goovaerts, J. De Sitter, J. Devreese: B.L.G., 439, Internal Report, Atomic Energy Center, Mol, Belgium (1969).

5. Finkenrath et al: Solid State Communications, 7, 11 (1969).

6. D. Larsen: Phys. Rev., 135, 1, 419 (1967).

7. Brown et al: in "Polarons and Excitons", Kuper editor, Oliver Boyd (1962).

8. Lax et al: Phys. Rev. Lett., 23, 1033 (1969).

9. Kobayashi et al: J. Phys. Soc. Japan, 28, 1096 (1970).

10. Gutzwiller: J. Math. Phys., 8, 1979 (1967).

11. C.C. Grosjean: Lecture presented at the Royal Flemish Academy (1970).

12. M. Goovaerts, J. Devreese: J. Math. Phys. (to appear May 1972).

13. Feynman: Phys. Rev., 97, 660 (1955).

14. Feynman et al: Phys. Rev., 128, 1599 (1962).

15. Thornber, Feynman: Phys. Rev. B. 1, 4099 (1970).